CASCADEX
- MODIFIED INTRANUCLEAR CASCADE AND EVAPORATION MODEL

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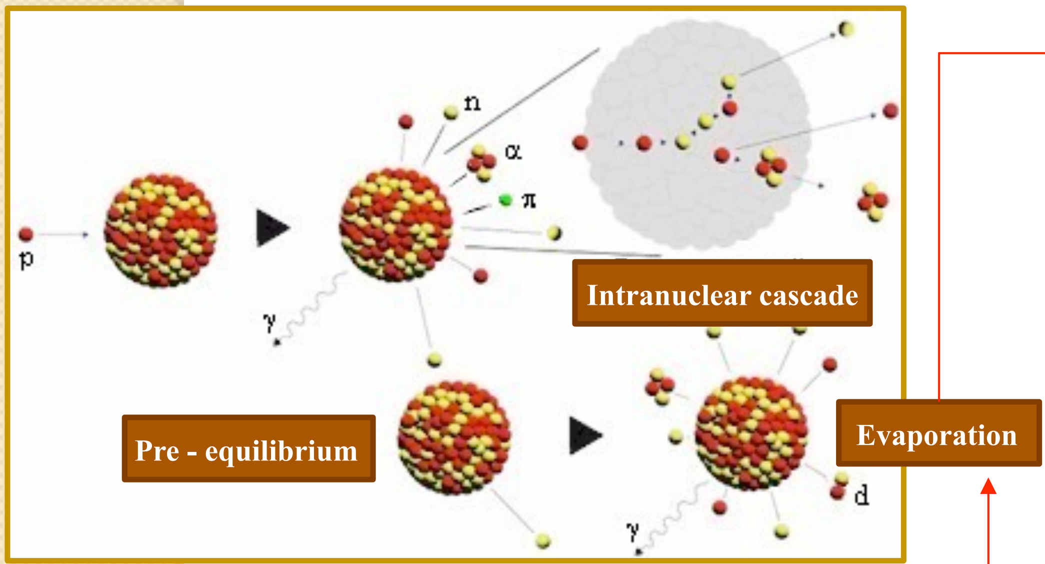
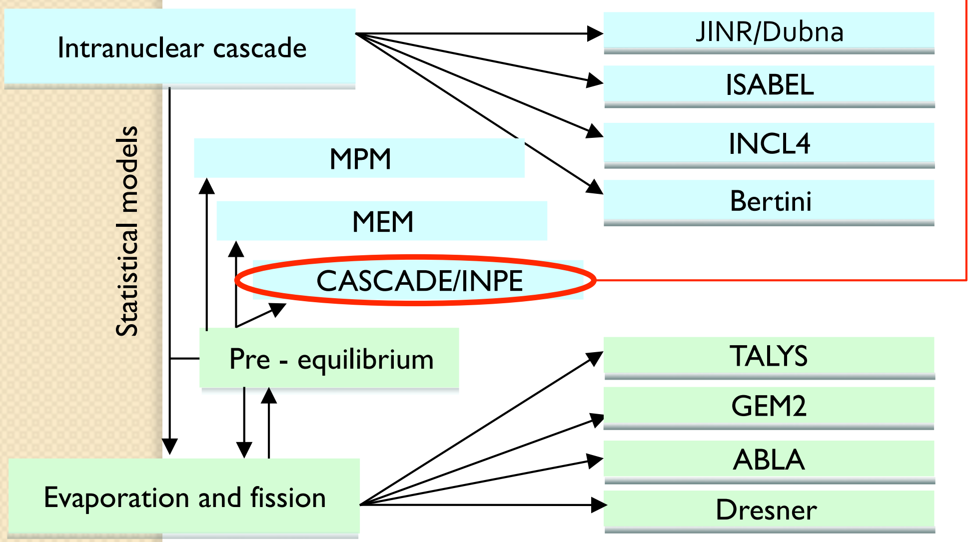
A.A. Natalenko, A.Yu. Stankovskiy

CONTENT :

Intranuclear cascade interactions scheme.

Usual approach





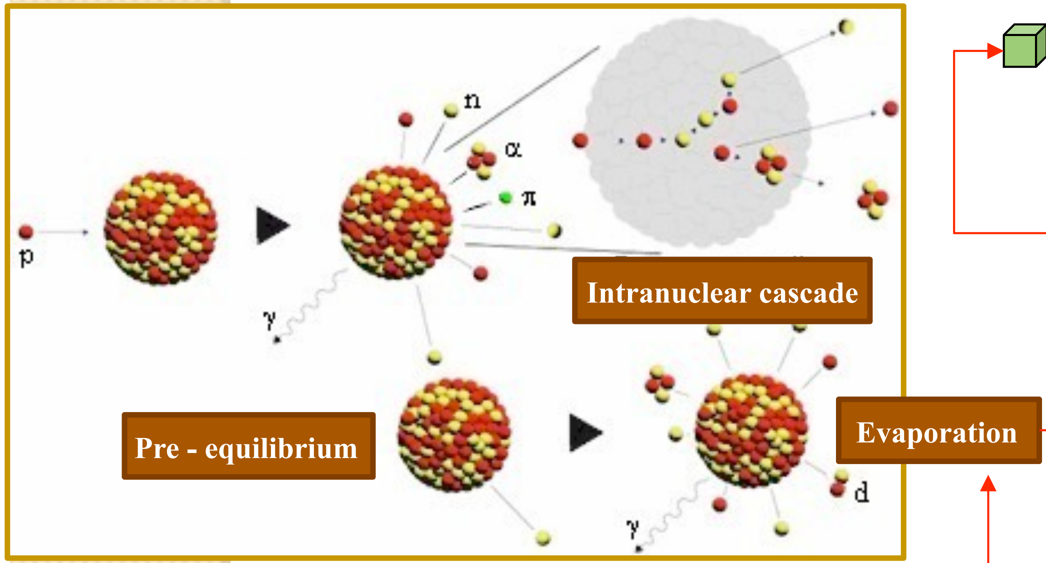
- Modern calculation codes use evaporation model based on a statistical phenomenological Weisskopf - Ewing approach.
  The Cross-Section in the Weisskopf-Ewing model is given by:

$$\frac{d\sigma}{d\varepsilon_b} = const\ \varepsilon_b \sigma_{inv}(\varepsilon_b) U^{-2} \exp(2\sqrt{aU})$$

where $a = (\pi^2/6)g$ – parameters of the level density (g - density of particle states near the Fermi energy), U - excitation energy of the final nucleus, ε_b - the energy of particle b, $\sigma_{inv}(\varepsilon_b)$ so-called inverse reaction cross-section.

* - V.F.Weisskopf, D.H. Ewing, Phys. Rev. 57 (1940) 472

Evaporation



Cross-section in the model of Hauser-Feshbach determined by the formula :

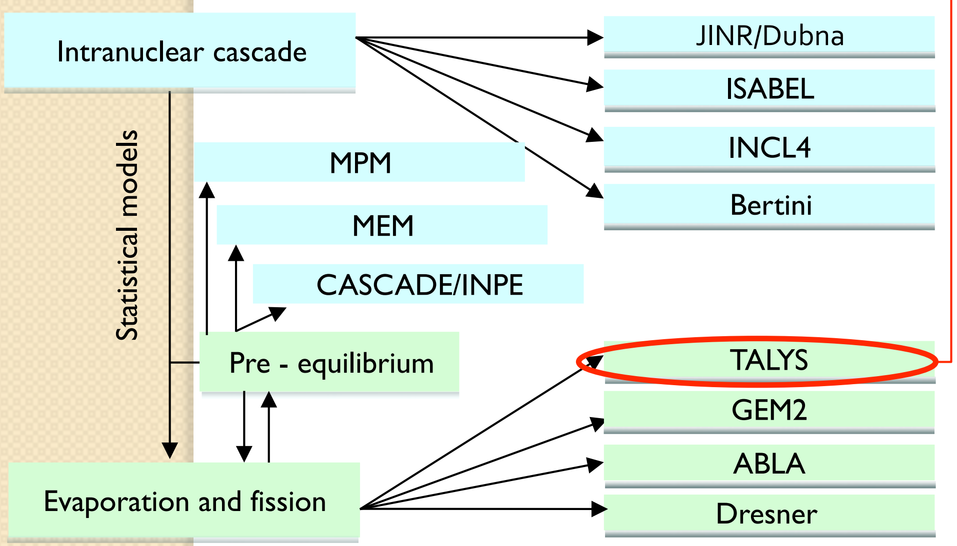
$$\sigma_{\alpha\beta} = \frac{\pi}{k_\alpha^2} \cdot \frac{T_\alpha T_\beta}{\sum_i T_i}$$

where T_α and T_β

$$\sum_{\beta \neq \alpha} |S_{\alpha\beta}|^2 = 1 - |S_{\alpha\alpha}|^2 = T_\alpha$$

In terms of average widths, this formula is as follows:

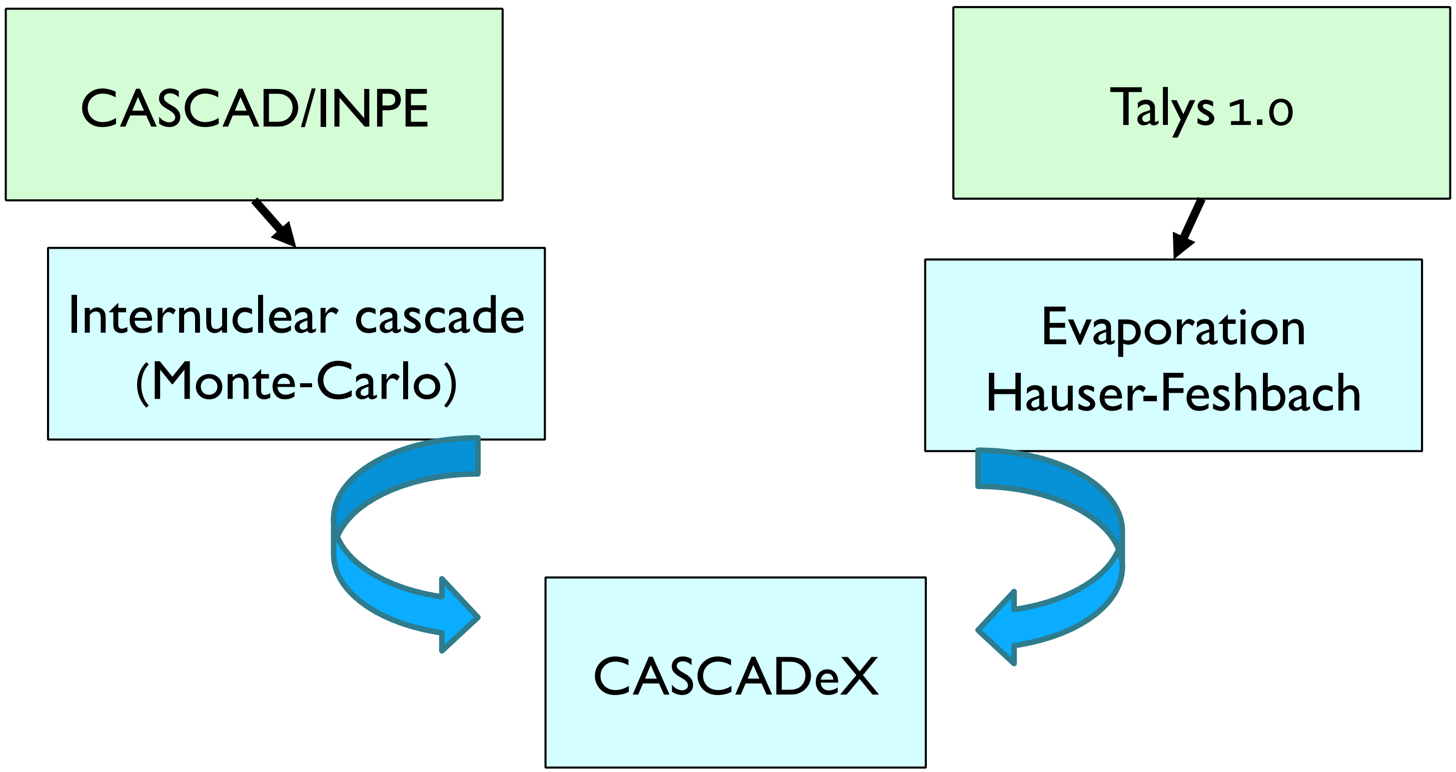
$$\sigma_{\alpha\beta} = \frac{\pi}{k_\alpha^2} \cdot \frac{2\pi}{D} \cdot \frac{\langle \Gamma_\alpha \rangle \langle \Gamma_\beta \rangle}{\langle \Gamma \rangle}$$



Hence to construct an evaporation model in the Hauser-Feshbach formalism the concept of scattering matrices is be used, which necessitates to know the type of bound and inverse cross-section. There remains the problem of S-matrix calculation, which is parameterized on the basis of the symmetry properties of the system.

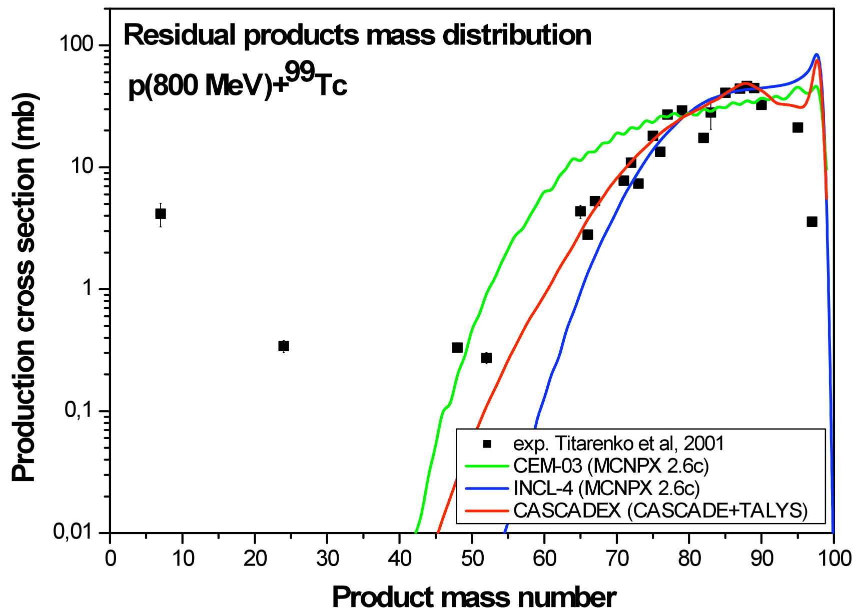
Idea behind CASCADEX

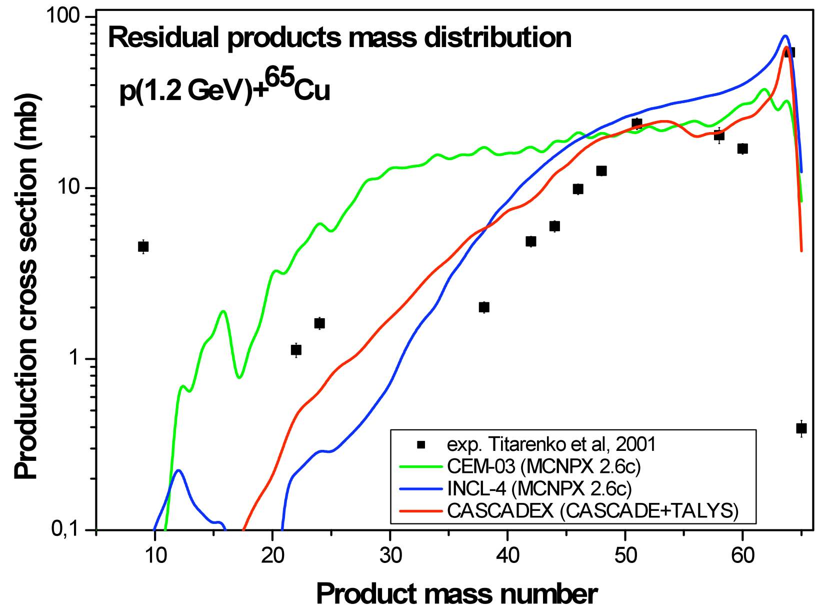
- *The fast intranuclear cascade stage follows by the de-excitation, which is described using the Hauser-Feshbach statistical model. The model proposed has been validated on radionuclide yields in proton-induced reactions at energies 0.8-1.2 GeV. The results show the advantages of using such approach instead of usual intranuclear cascade and evaporation algorithms.

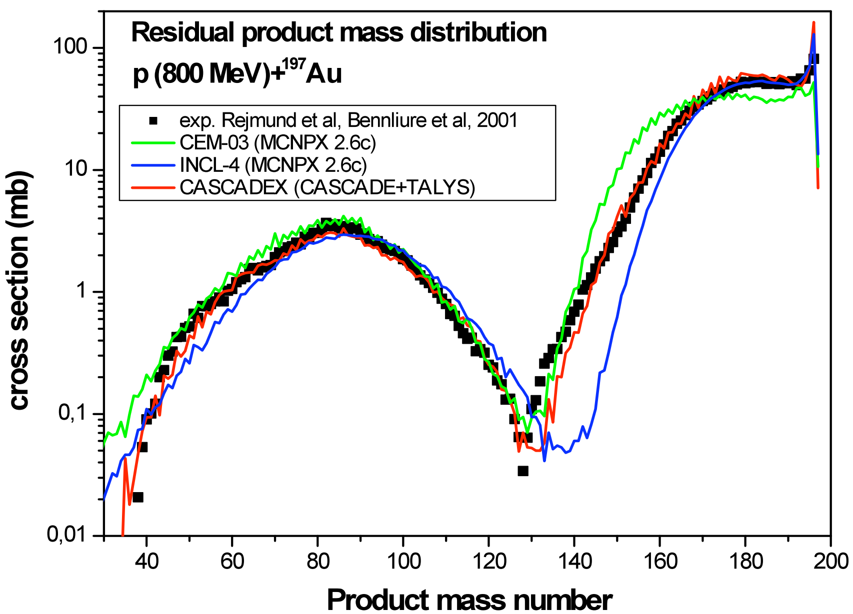


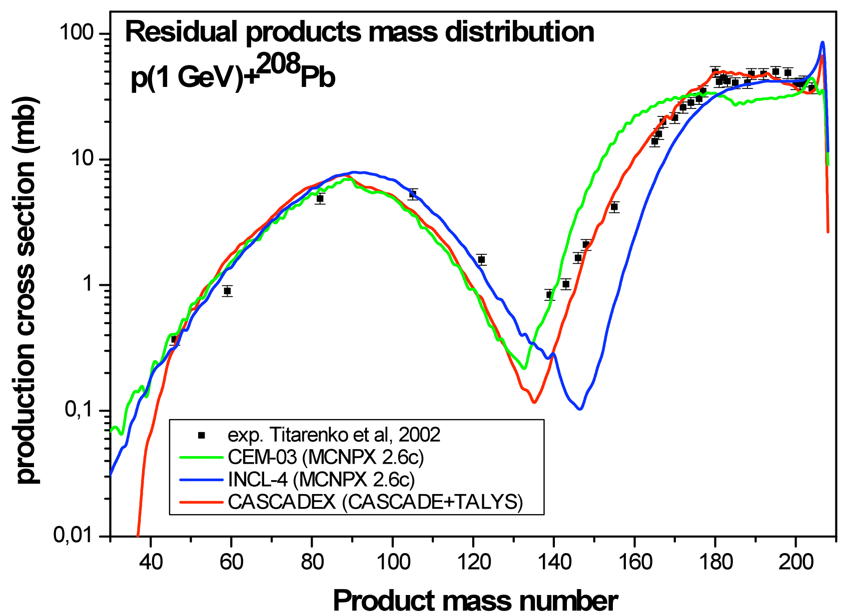
* - W.Hauser and H.Feshbach, Phys.Rev. 87 (1952) 366.
- A.J. Koning, S. Hilaire and M.C. Duijvestijn, Proc. Int. Conf. on Nuclear Data for Science and Technology -ND2004, AIP vol. 769, eds. R.C. Haight, M.B. Chadwick, T. Kawano, and P. Talou, Sep. 26 - Oct.1, 2004, Santa Fe, USA, p. 1154 (2005).

verification CASCADEX (I)

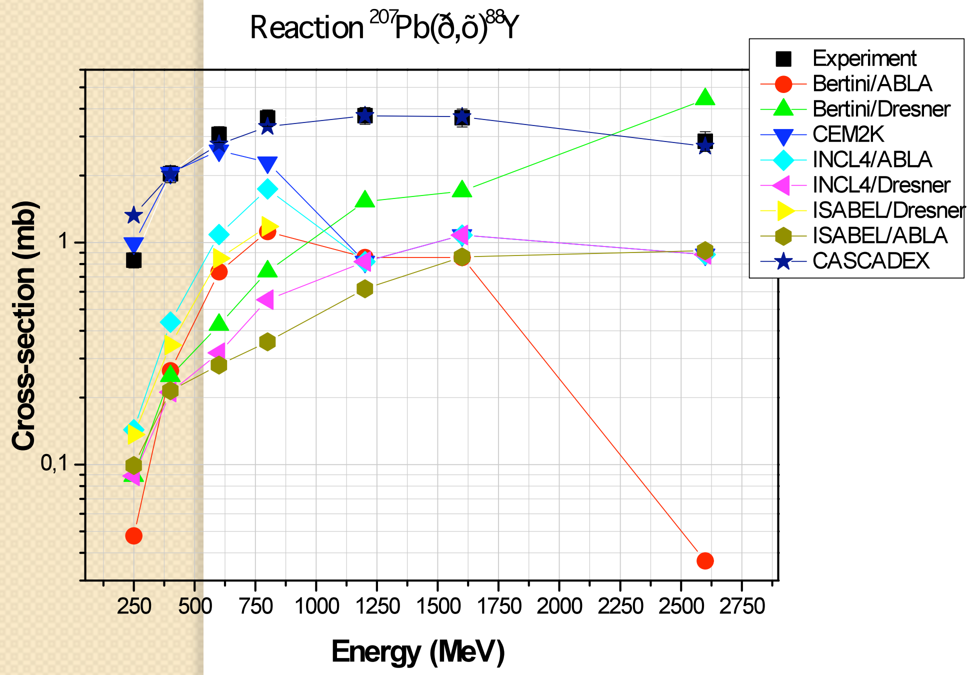


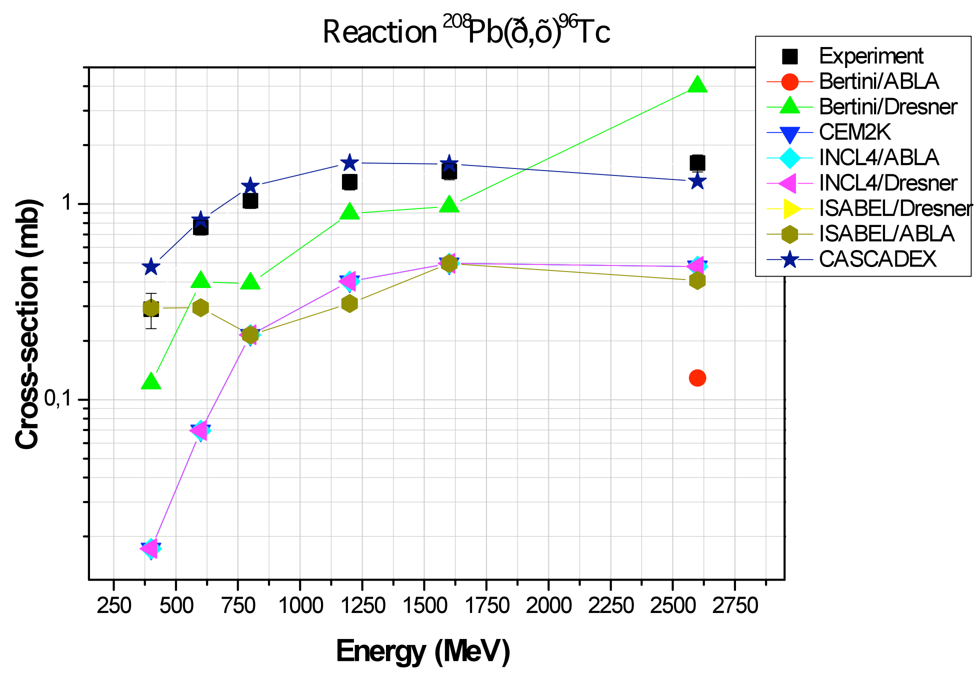


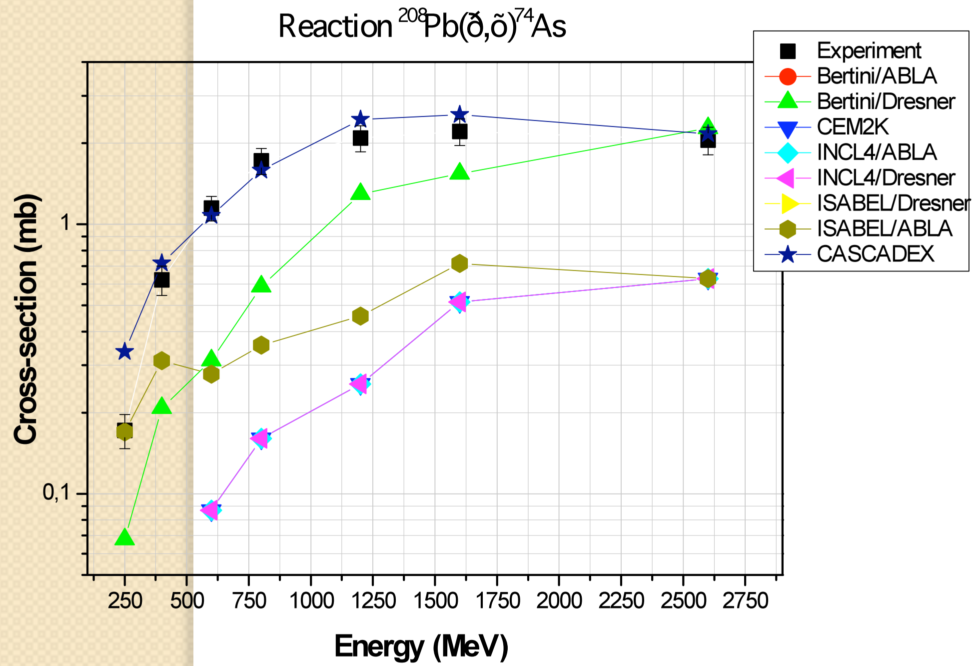


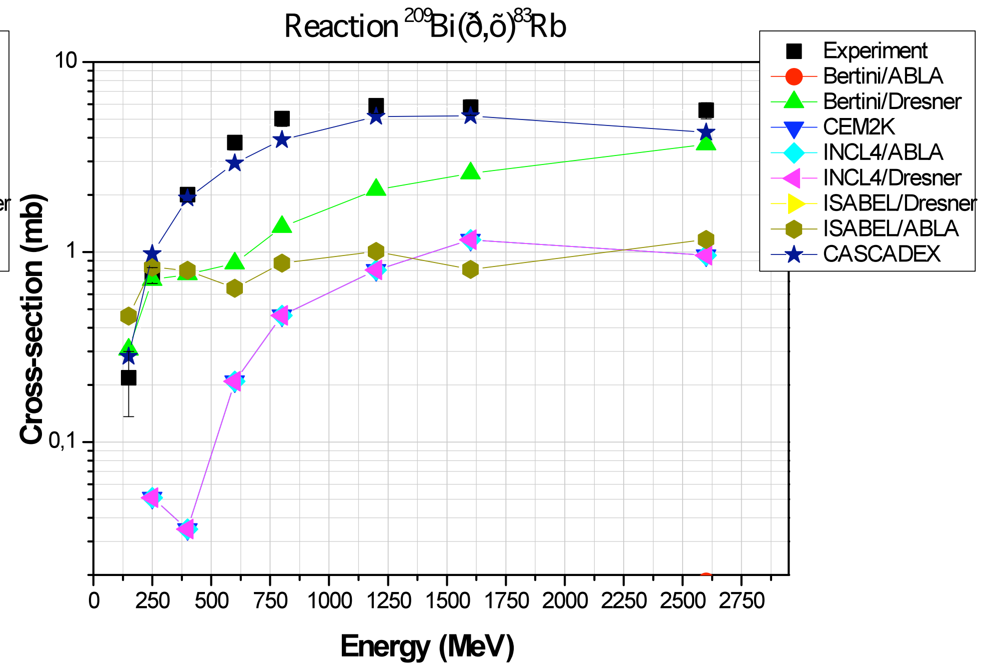


verification CASCADEX (2)

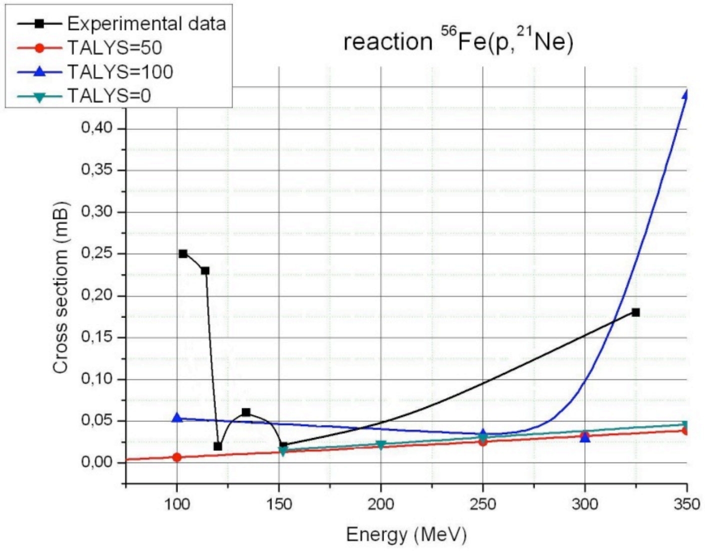


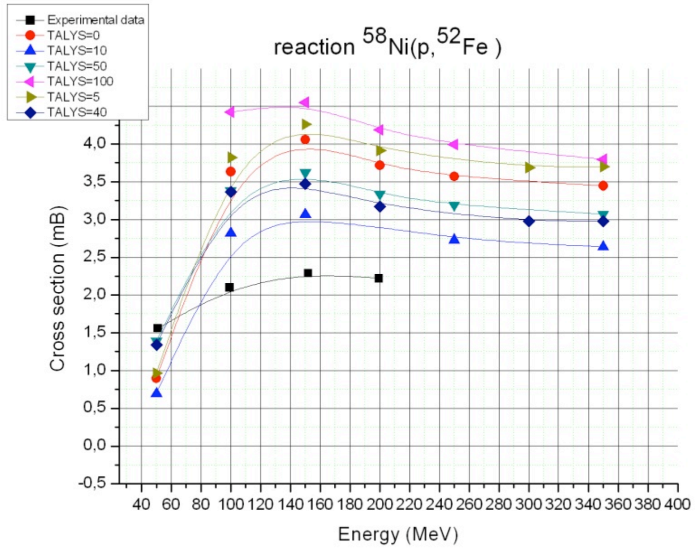


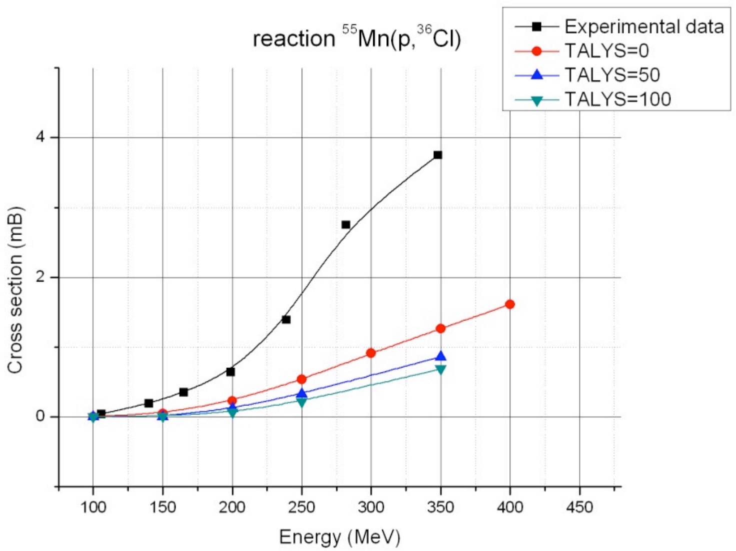


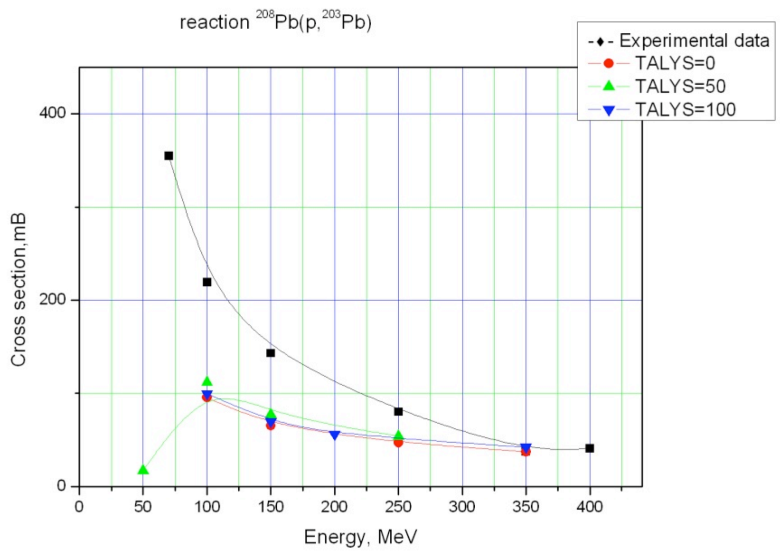


Assessment of threshold energy between fast stage and de-excitation









HOW TO RUN CASCADEX CODE

Distribution (I)

- The CASCADEX code has been tested under Windows and Linux on different compilers. Under Windows, the Compaq Fortran complier v.6.x or Intel Fortran complier 9.x is needed. Under Linux, the Intel Fortran complier v.9.x or G95 has to be used to compile or execute the code.
- In the package you will find the file install.bat (necessary to install under windows) or install.sh (linux bash shell script). Open corresponding file (install.bat or install.sh). Modify the parameter fcomp= corresponding to the Table below. The table contains list of compilers for which the installation and run of CASCADEX is guaranteed.

Fortran Compiler	Parameter fcomp under Windows	Parameter fcomp under Linux
G95	set fcomp=g95	fcomp=g95
Intel Fortran	set fcomp=ifort	fcomp=ifort
Comaq Visual Fortran v. 6.x	set fcomp=cvf	-

- Modify the parameter talyspath=. The path has to include the name of TALYS executable already installed on your machine.
- Also on windows system you must to indicate the “structure” folder of Talys program in toptions.ini

Distribution (2)

File name	Description
cascadex	Binary executable of the code. To run it, Intel Fortran should be pre-installed and the command **chmod a+x cascadex** has to be run before executing.
catalys	The talys 1.0 binary executable created also with Intel Fortran. The same command **chmod a+x catalys** should be supplied before running the executable. **Attention!** *The directory STRUCTURE with the data files necessary to run talys has to be placed at the same level as this executable.* **RECOMMENDATION.** *If the talys 1.0 executable already exists somewhere, it should be copied in the directory of CASCADEX with the name CATALYS (only this file name is supported by CASCADEX).*
Comp.sh	Shell script to compile CASCADEX
input	Input file for CASCADEX. Do not rename this file.
Cascadex.f	Main source file of CASCADEX
Readgeneralinput.f	Subroutine reading input file. Called by Cascadex.f
Excmass.f	Subroutine preparing the mass table for cascade. Called by Cascadex.f
Barriers.f	Subroutine preparing the fission barriers for cascade. Called by Cascadex.f
Docasc.f	Subroutine invoking the intranuclear cascade model. Called by Cascadex.f
Runtalys.f	Subroutine invoking the CATALYS executable. Called by Cascadex.f
Writeresults.f	Writing results to output files. Called by Cascadex.f
Inelaa.f, evapor.f, deltam.f, delen.f, barash-sigion.f, basics.f, time.f, pauli.f, urand.f	Subroutines of CASCADE code. Called by docasc.f

Description of input file

Name of the file: input. Only this name is supported at the moment. Consisits of 8 free-format lines. All of them are described inside the file:

- Line 1: incident particle: 1-p, 2-n, 3,4,5 - pions,6,7-muons,8-d,9-t,10-he3,11-a
- Line 2: incident particle energy in MeV
- Line 3: target charge and mass numbers
- Line 4: Energy below which TALYS is invoked. Typically – 200 MeV (the maximum energy mentioned in the TALYS manual). If 0 MeV is entered, only cascade code is invoked and evaporation follows Weisskopf-Eving scheme.
- Line 5: Statistics for cascade. Current memory restrictions do not allow the values higher than **20 millions** of cascade histories. These limitations should be turned off in the future.
- Line 6: flag for enabling/disabling fission in talys. If fission in talys is disabled, the fission is handled by cascade.
- Line 7: flag for restart of talys. Typically, the calculation lasts from hours to days, and there is a risk to loose results in case of hardware accident. For that, user can restart talys calculation from the last successfully processed compound nucleus (it should be noted here, that compound nuclei are processed in ascending order – from low A to high A).
- Line 8: an and af values to tune residual products mass distributions. It is recommended to run single cascade first (value in Line 2 = 0) to estimate the necessary an and af values, and after that to run complete CASCADEX cycle (with the value in Line 2 e.g. 200 MeV) to get better results.

Output files

File	Description
Resid_c.dat	File produced after cascade stage. Contains information on residual nuclides after this stage: Z,A, yield (nuclei/primary particle), cross section (CS=Y*nonelastic CS).
Mc_distr.dat	Mass distribution of residuals after cascade stage. Contains A, yield and cross section.
Residuals.dat	Residual products after each cycle of talys run (number of talys runs = number of compound nuclei produced by cascade).
Massdistr.dat	Mass distribution of residuals after each talys run.
Residfin.dat	Final residual products file created after last talys run.
Mdfin.dat	Final mass distrib ution after last talys run.
Fptalres.dat	Fission products produced in talys run, if the fission in talys was requested in input.
Fptalmas.dat	Mass distribution of fission products after talys, , if the fission in talys was requested in input.
beforetalys	Temporary binary file needed for restart of talys (analog of runtpe file in mcnp/mcnpx).
*.no, *.po	Double differential cross-section of protons and neutrons
*.do, *.to, *.ho, *.ao	Double differential cross-section of light particles

CASCADEX – MODEL INGREDIENTS AND PARAMETERS

Parameters of first stage model (INC) (1)

N-N interaction elastic and inelastic cross-section	1) N-N interaction elastic: Yes 1) Inelastic cross-section calculated using INC model [1-3]: Yes [1] V.S. Barashenkov, et al., Nucl. Phys. A 338 (1980) 413. [2] V.S. Barashenkov, Comput. Phys. Commun. 126 (2000) 28. [3]V.S. Barashenkov, Nucl. Phys. A 231 (1974) 462.
Nuclear medium description	Continuous medium Woods-Saxon
In medium corrections of N-N interaction	Yes.
Nuclear average potential (V_N, V_π)	It is assumed that nucleons are located inside the potential well: $V(r) = \xi + \frac{P_f^2}{2m}$ Where m is the mass of nucleon, ξ the average binding energy of nucleon in the nucleus and P_i the nucleon momentum inside the nucleus.
Nuclear shape description	Sphere with radius $R = 1{,}07 A^{\frac{1}{3}}$ fm. Woods-Saxon.
Production of composite particles during the cascade stage or not. If yes, parameters of the coalescence mechanism description	Coalescence model [4] P_0 varies for the different nuclei. For example P_0=330 for ^{208}Pb and for ^{56}Fe is P_0=170-230 depending on the projectile energy. [4] T.C. Awes Light particle emission in ^{16}O-induced reaction at 140, 215, and 310 MeV

Parameters of first stage model (INC) (2)

Implementation of the Pauli blocking and related parameters	Pauli blocking implemented.
Pre-equilibrium or no. If yes, parameters of the pre-equilibrium model, criterion to switch from INC to pre-equilibrium and from pre-equilibrium to de-excitation	No
If no-pre-equilibrium, criterion to switch from INC to de-excitation	The INC part ‘‘piles up’’ some population after the fast stage depending on the ‘‘threshold’’ energy, below which de-excitation will be handled by TALYS. This energy of excited nucleus after INC stage is the model parameter. It may vary from 0 to 200 MeV.
Range of validity in energy and mass	The range of INC model validity: The range of projectile mass numbers is up to 240, the target material mass range is from 2 to 240. The projectile energies might be up to 2 GeV/nucleon for targets with mass number below 40 and up to 1 GeV/nucleon for targets with mass number above 40. However, if the mass and energy of excited nucleus after INC stage exceed the TALYS limits (mass 12 and higher, energy 1 keV-200 MeV), this nucleus is not considered.
Computational time (time per event for a typical case and indication of the platform)	INC phase – very fast, Comparable with other models. De-excitation phase is handled by TALYS so it is slow. Typical calculation time for 1 GeV protons of ^{208}Pb - 1 day on 3 GHz PC with INC calculation takes less than 1 hour.

Parameters of de-excitation models

level densities	Constant temperature + Fermi gas model (Talys Default model) [1] [1] Talys manual. Page 83.
Inverse reaction cross-sections: σ_{inv} including Coulomb barriers for the different types of evaporated particles	Inverse reaction cross section calculated with the optical model [2] [2] TALYS manual. Page 54
Fission barriers	The fission barriers were taken from A.J. Sierk, Phys. Rev. C33 (1999) 2039
Fission fragment generation	The distribution of fission fragments is calculated according to A.Yu. Konobeyev, Yu.A. Korovin, M. Vecchi, Kerntechnik 64 (1999) 216.
List of de-excitation channels and related parameters	Competition of fission, particle and photon emission. (Talys manual p .79)
Capability of the model to handle isomers	Generally no(even if TALYS can handle, INC stage does not produce metastable nuclei)

BENCHMARK OF SPALLATION MODELS

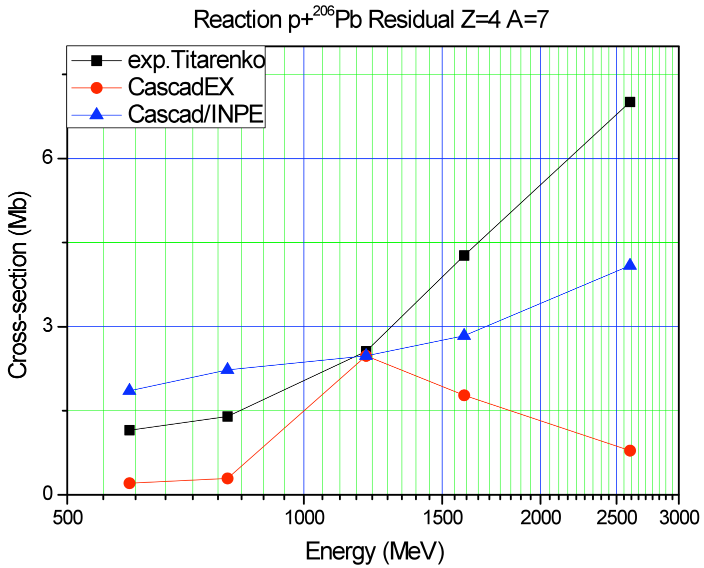
Production cross-sections

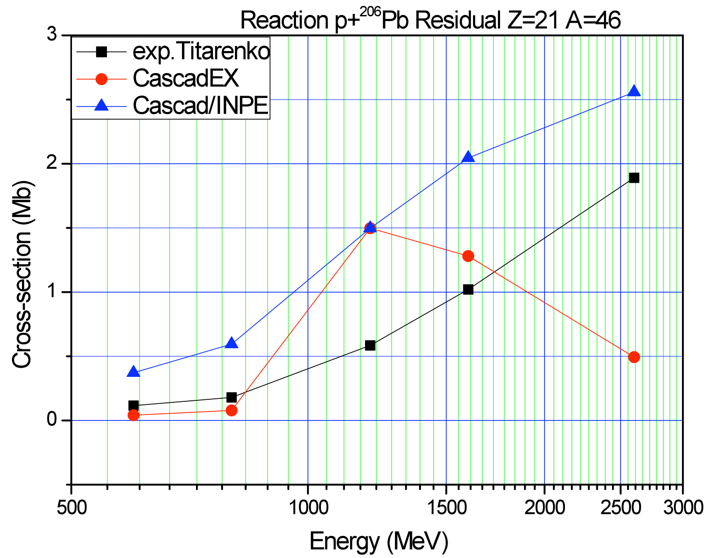
Production cross-sections from threshold to 3 GeV (excitation functions)

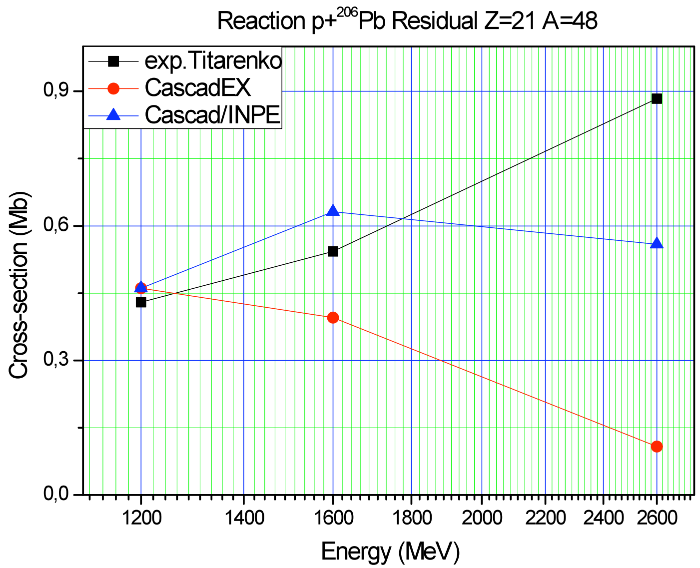
Beam	Target	Energy [MeV]	Laboratory	Reference	Data
p	Fe	20 to 3000	Hannover University, Germany University of Bern, Switzerland ITEP, Russian Federation	R. Michel et al., Nucl. Sci. Tech., Supplement 2 (2002) 242 - K. Ammon, I. Leya et al., Nucl. Instr. and Meth. B 266 (2008) 2 - ▪ R. Michel et al., Nucl. Instr. and Meth. B 103 (1995) 183 -; ▪ Th. Schiekel, R. Michel et al., Nucl. Instr. and Meth. B 114 (1996) 91 -; ▪ R. Michel et al., Nucl. Instr. and Meth. B 129 (1997) 153 - Titarenko (soon, october 2008?)	data | figure data | figure ▪ data | figure data | figure
p	Pb	20 to 3000	ITEP, Russian Federation ETH Zürich, Switzerland Hannover University, Germany	Y. E. Titarenko et al., Nucl. Instr. and Meth. A562 (2006) 801 - M. Gloris et al., Nucl. Instr. and Meth. A463 (2001) 593 - I. Leya et al., Nucl. Instr. and Meth. B229 (2005) 1 -	data | figure data | figure data | figure

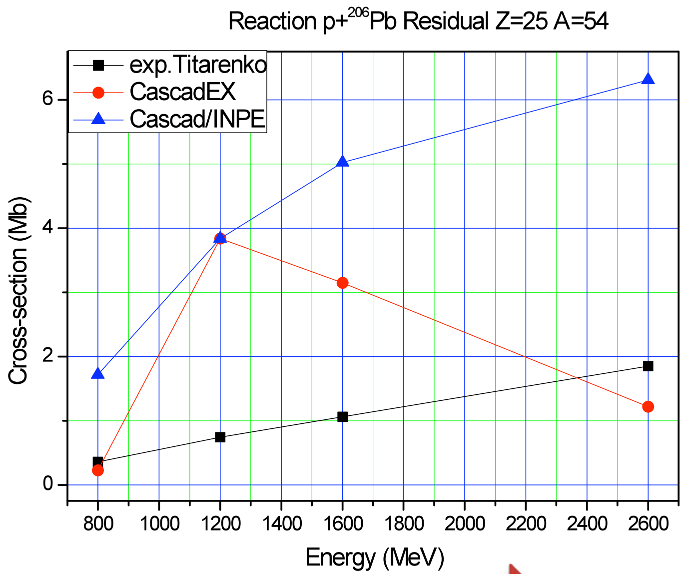
http://nds121.iaea.org/alberto/mediawiki-1.6.10/index.php/Benchmark:ExpDataSets

Light spallation products



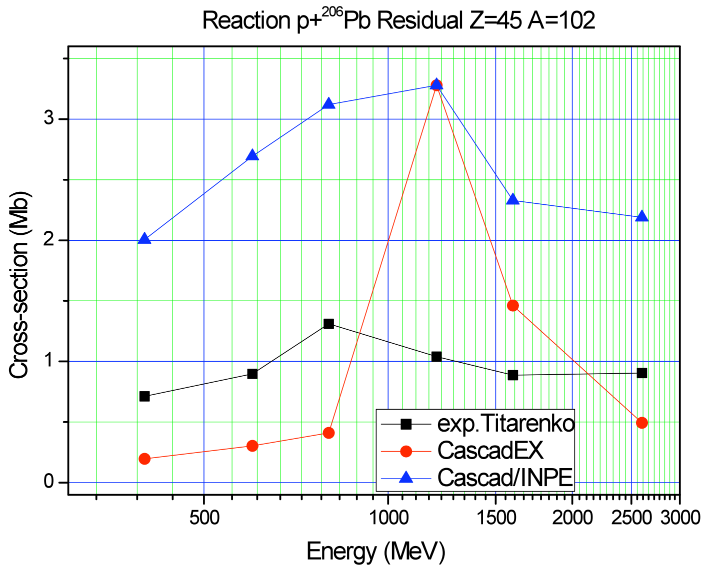


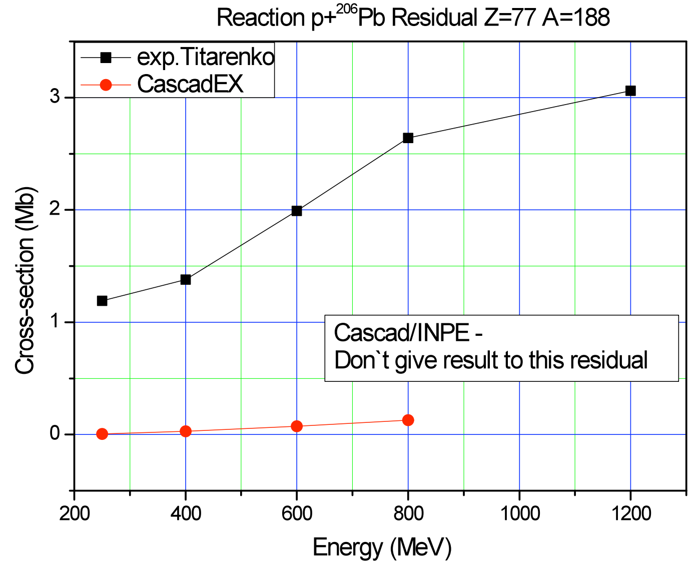


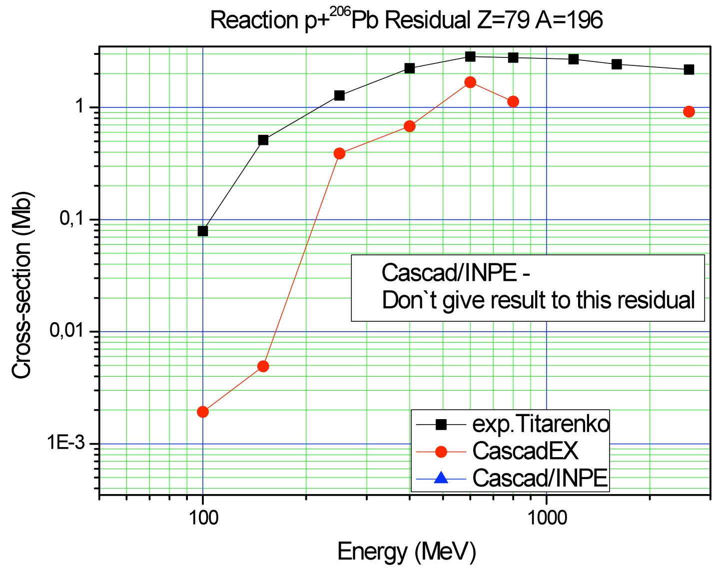


Increasing Z,A of spallation products

Intermediate spallation products

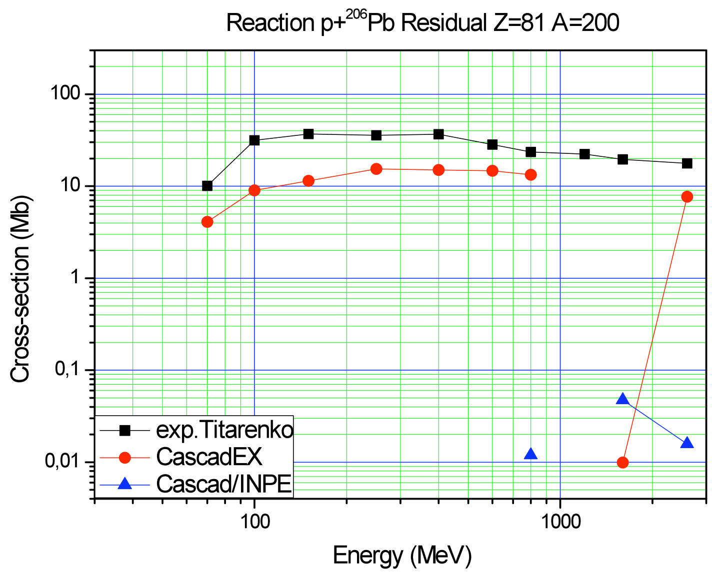


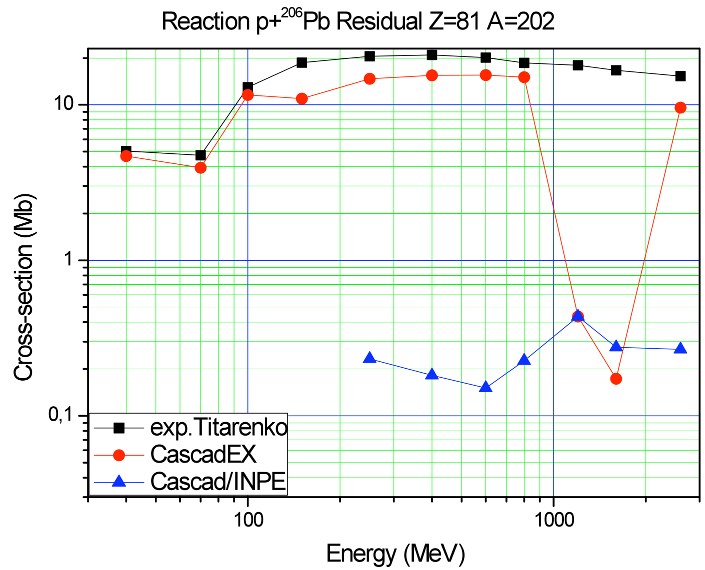


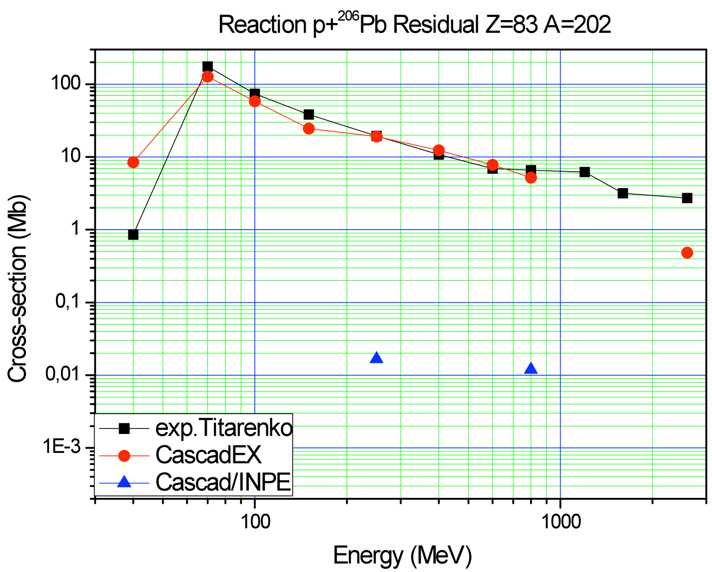


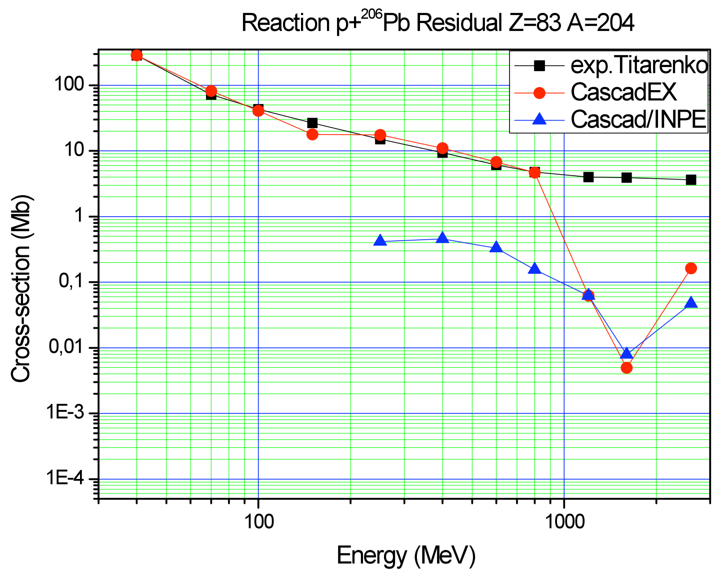
Increasing Z,A of spallation products

Heavy spallation products



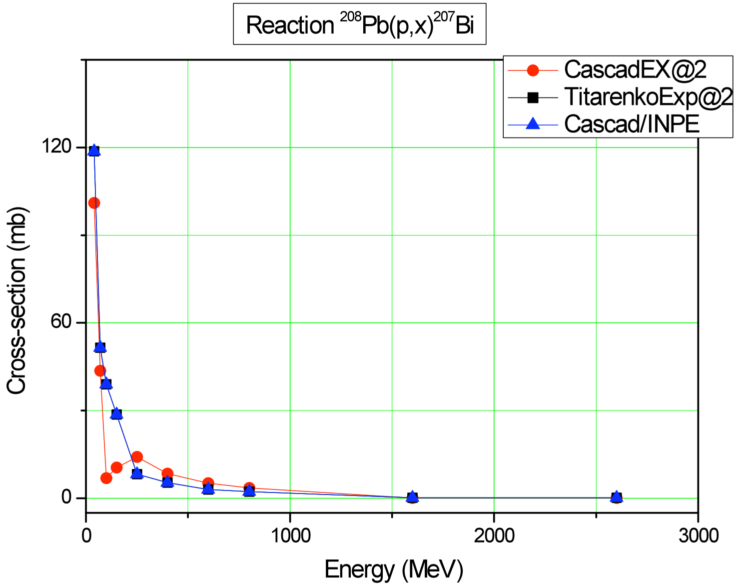


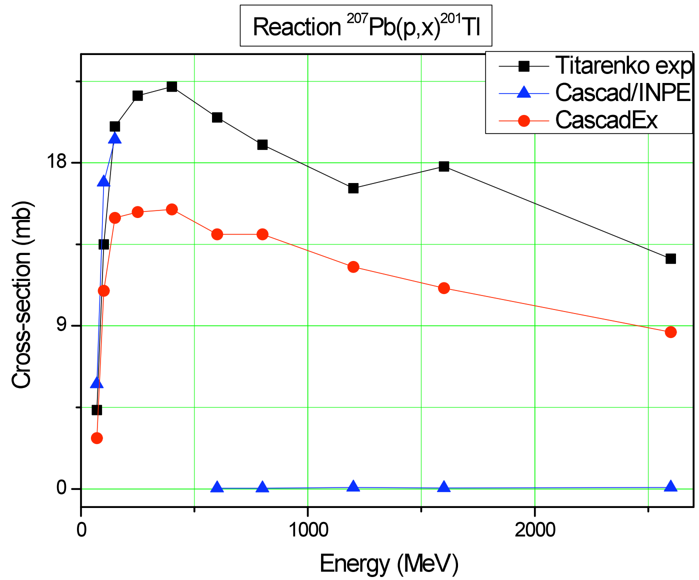


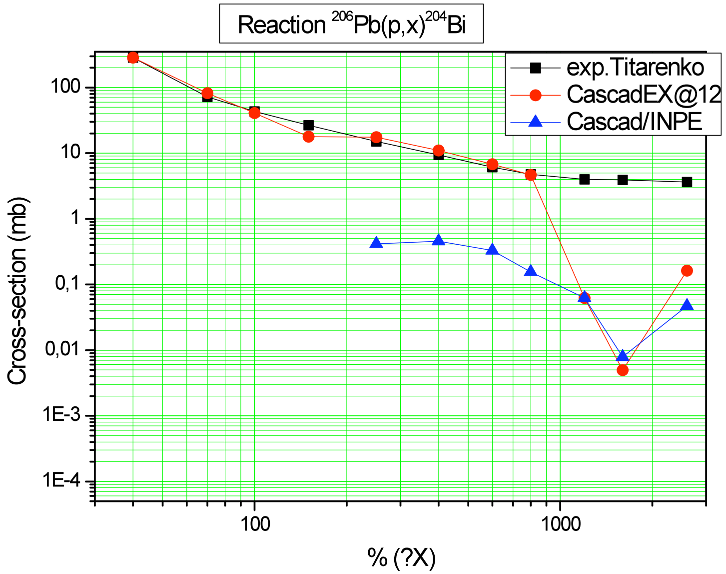


Increasing Z,A of spallation products

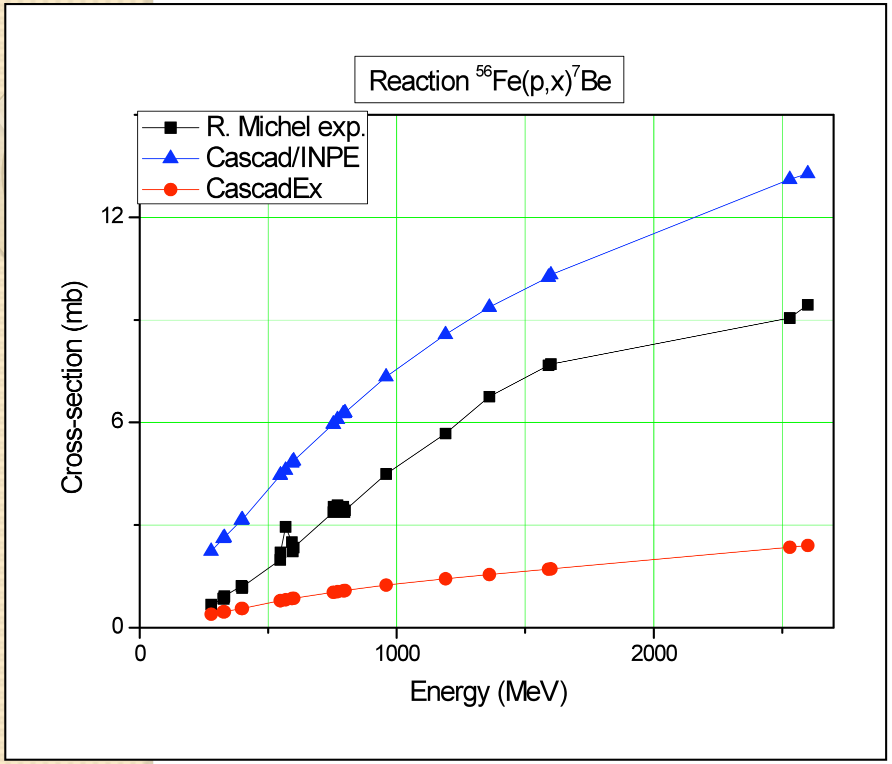
Benchmark of data for Pb

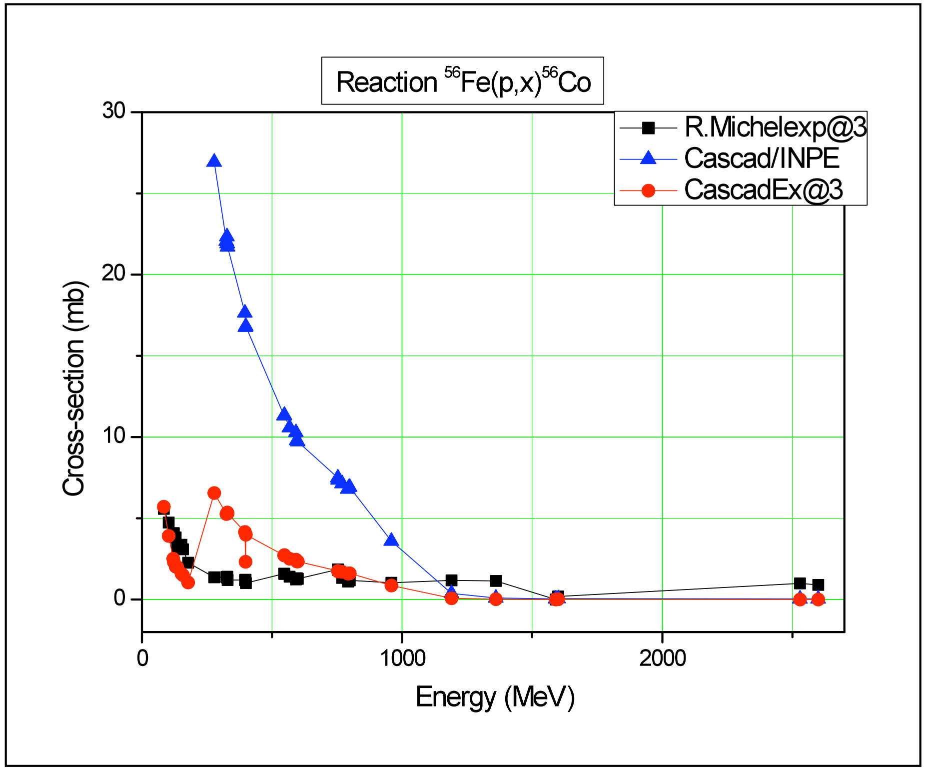






Benchmark of data for ^{56}Fe





LIGHT CHARGED PARTICLE PRODUCTION

Double Differential Cross-Section Calculation using CascadEx Code

Moving Source Model:

$$\frac{d^2N}{d\Omega dE} = N_0 \cdot \sqrt{E_{ac}} \cdot \exp\left(\frac{[-E - Z \cdot E_c + E1 - 2 \cdot \sqrt{E1} \cdot \sqrt{E_{ac}} \cdot \cos(\theta)]}{T(\theta)}\right)$$

,where

$$T(\theta) = T_0 \cdot \exp(\frac{-\theta}{45.5})$$

- N_0- normalization constant for each spectrum
  E_{ac}=E-ZE_c – is the energy before acceleration in the Coulomb field.
  E_c- the Coulomb energy per unit charge
  Z – the charge of the emitted particle
  E1=mV^2 /2 – kinetic energy of the particle of mass m at rest in the center of mass frame moving at velocity V

T.C. Awes Light particle emission in ^{16}O-induced reaction at 140, 215, and 310 MeV // Physical review C volume 25, Number 5

Double Differential Cross-Section Calculation using CascadEx Code

Coalescence model:

$$\frac{d^2N(Z,N,E_A)}{dE_A d\Omega} = \left(\frac{N_t+N_p}{Z_t+Z_p}\right)^N \frac{A^{-1}}{N!Z!}\left\{\frac{\frac{4}{3}\pi\cdot P_0^3}{\left[2\cdot m_0^3\cdot(E-E_C)\right]^{\frac{1}{2}}}\right\}^{A-1}\cdot\left\{\frac{d^2N(1,0,E)}{dE d\Omega}\right\}^A$$

N_t, N_p and Z_t, Z_p are the neutron and proton numbers of target and projectile respectively
m_0 – is the nucleon rest mass
$d^2N(Z,N,E_A)/dE_A\, d\Omega$ – differential multiplicity of nuclei composed of Z protons and N = A-Z neutrons
E_A=AE-NE_c, where E_c- is the Coulomb repulsion per unit charge
P_0 – coalescence radius

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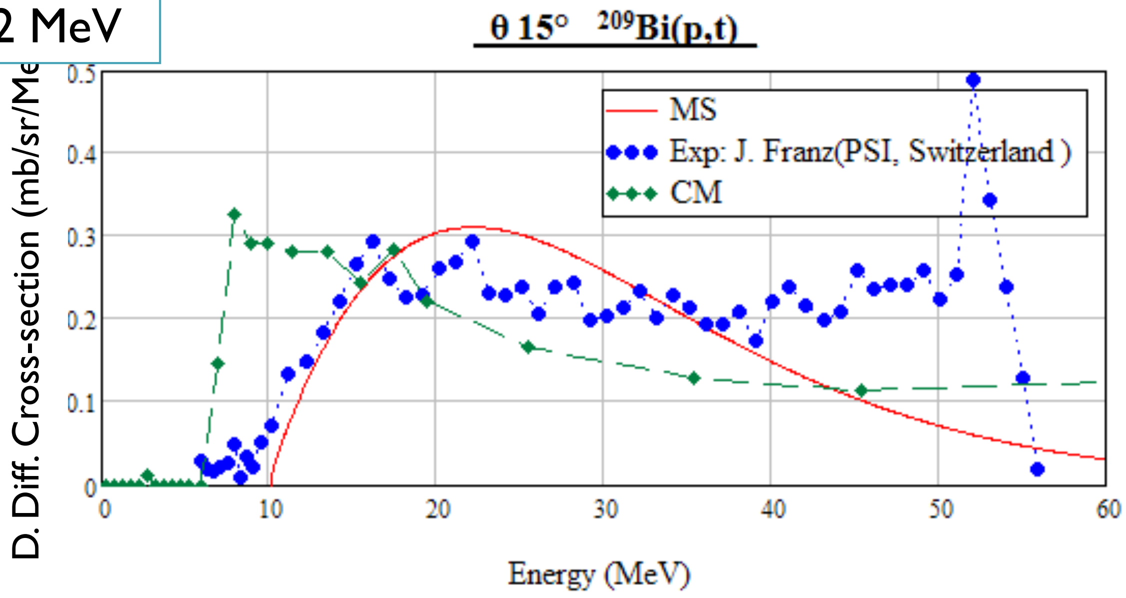
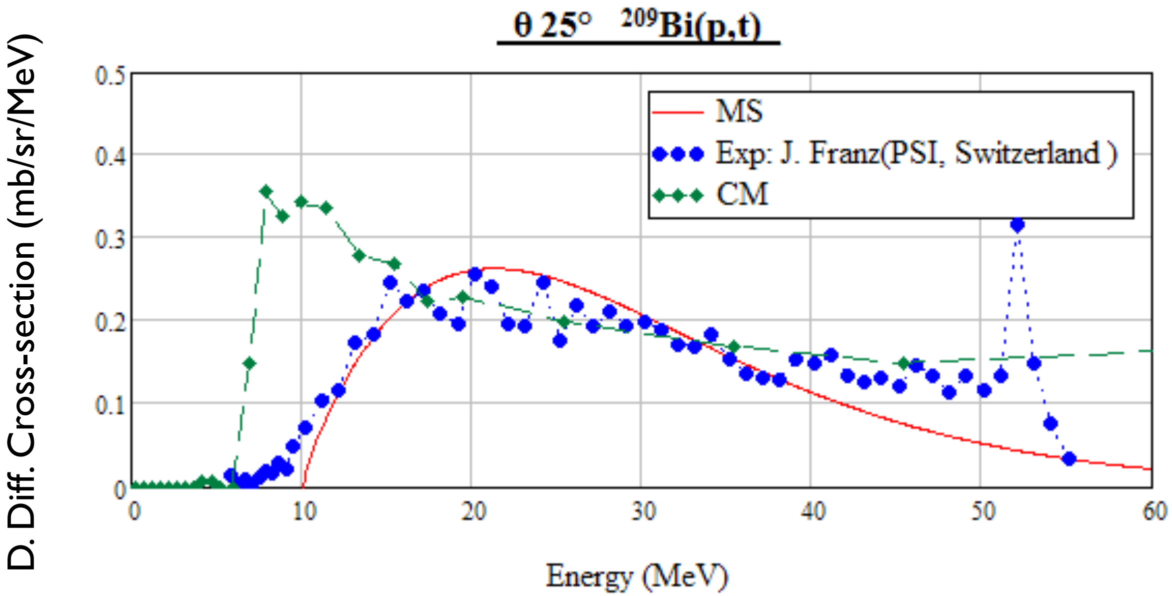
Intercomparison of moving source and coalescence models

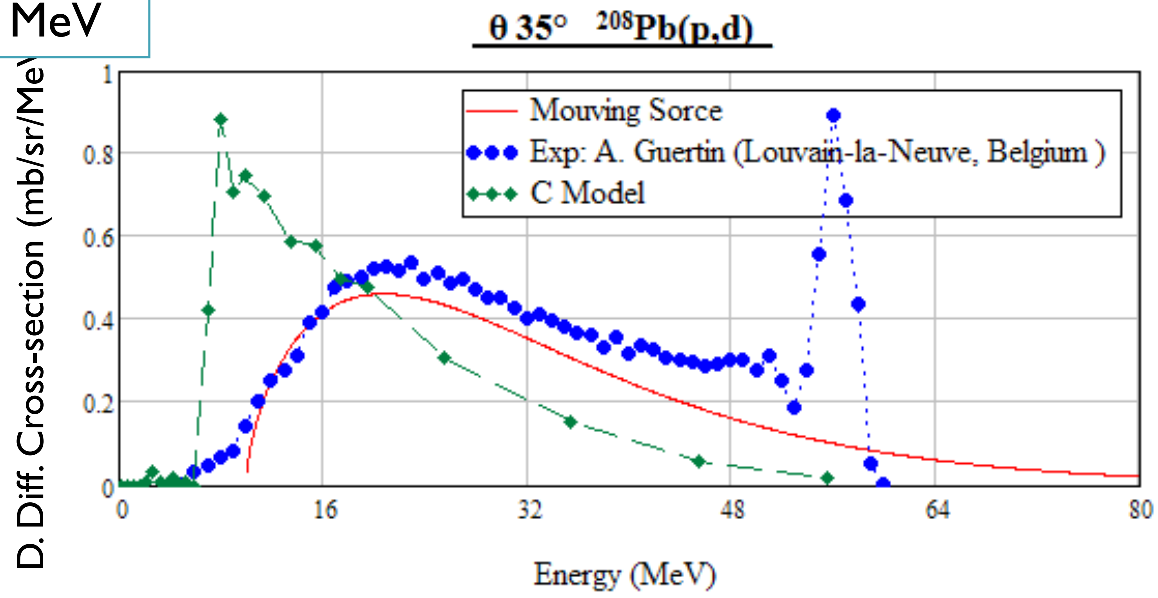
Projectile Energy = 542 MeV

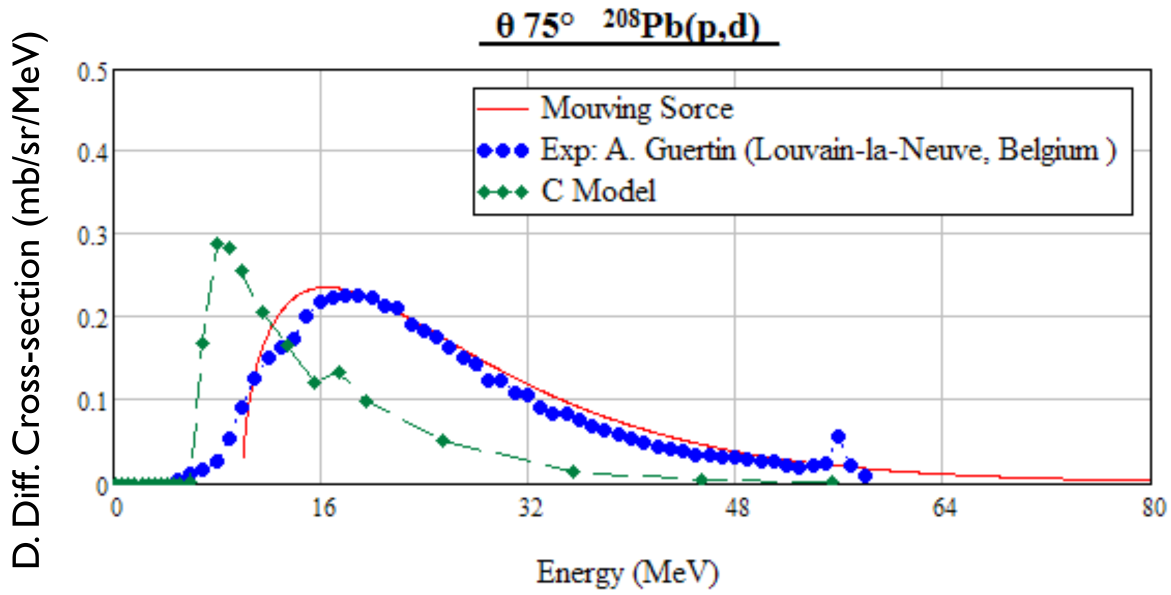




Intercomparison of moving source and coalescence models

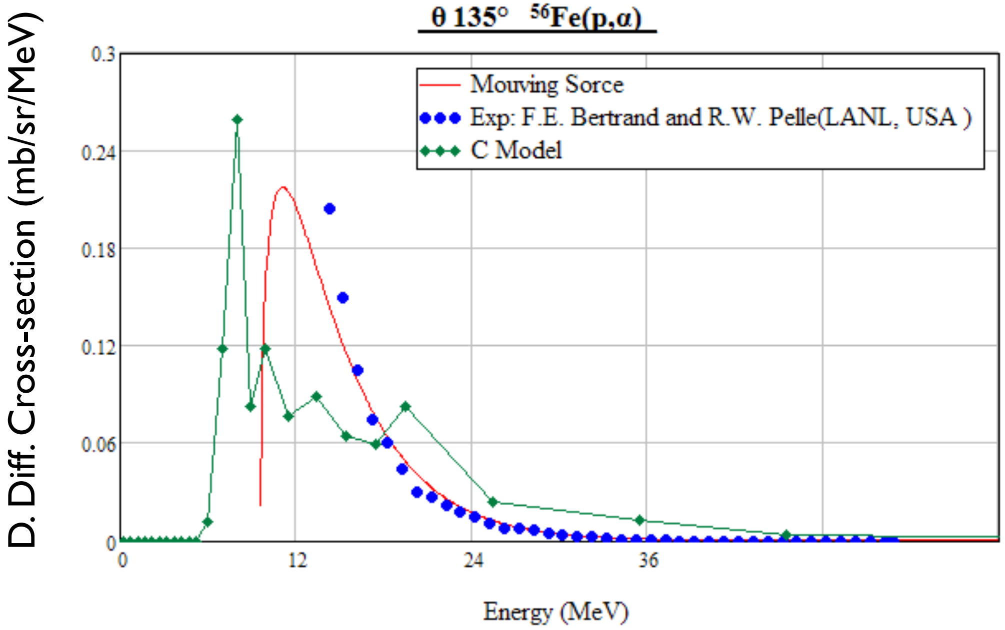
Projectile Energy = 63 MeV

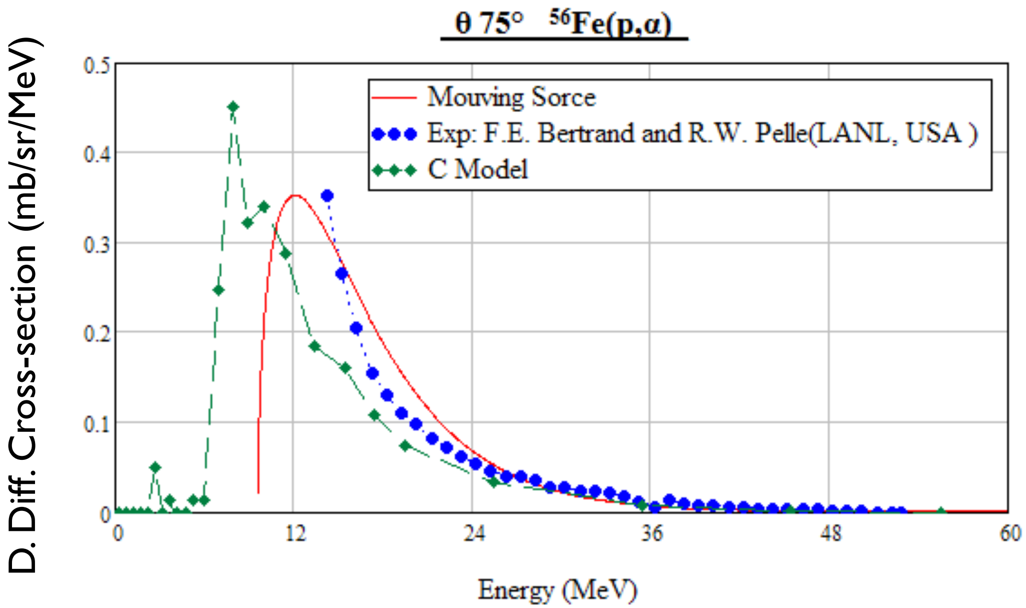




Intercomparison of moving source and coalescence models

Projectile Energy = 62 MeV





HIGH ENERGY ACTIVATION DATA LIBRARY

High Energy Activation Data Library

HEAD-2009 CONTENT

High Energy
Proton Activation Data
(HEPAD-2008)
Total isotopes – 682 (Z=1-84)

High Energy
Neutron Activation Data
(IEAF-2005)
Total isotopes – 682 (Z=1-84)
+ Update IEAF-2005-rev1-2009
(39 isotopes)

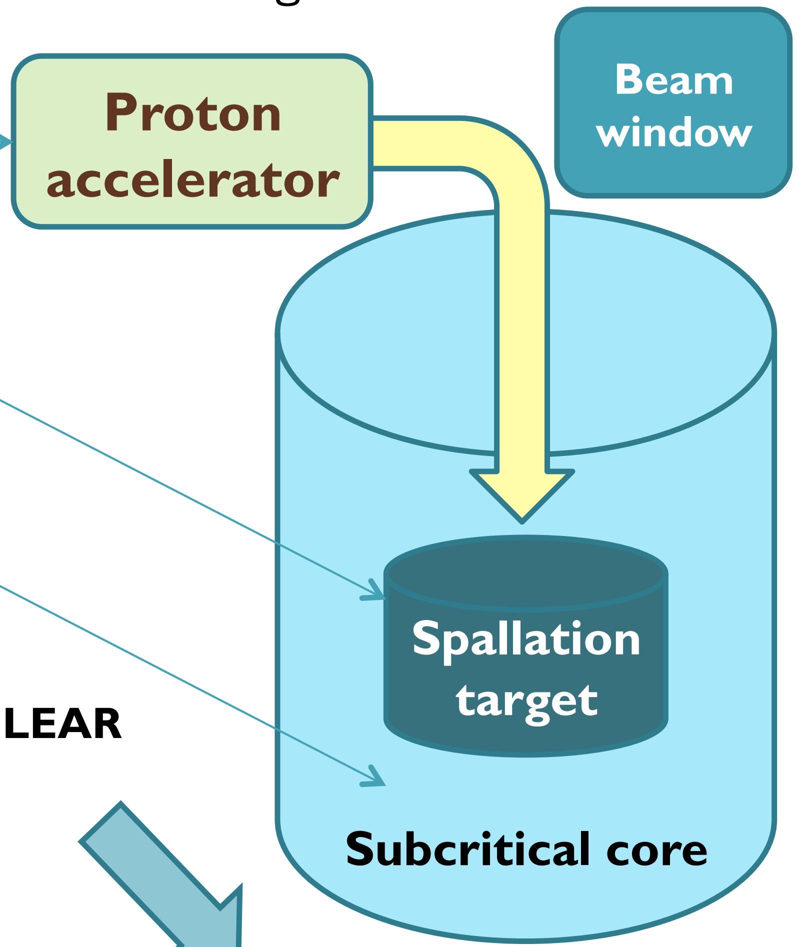
Energy range: from 150 MeV to 1 GeV (33 points)

ENDF-6 format: MF=3 MT=5 Non-elastic cross sections
MF=6 MT=5 Isotope production cross sections

HEAD-2009 APPLICATION

Accelerator Driven Transmution Technologies

- Accelerator technology
- Spallation target technology
- Subcritical reactor aspects



HIGH ENERGY ACTIVATION NUCLEAR DATA (IN GENERAL UP TO 1 GEV)

TARGET:

• Spallation products accumulation;

•Power density distribution.

COOLANT:

•Activation

BEAM WINDOW:

•Neutron and proton transport;

•Radiation material damage.

EVALUATED ACTIVATION NUCLEAR DATA LIBRARIES

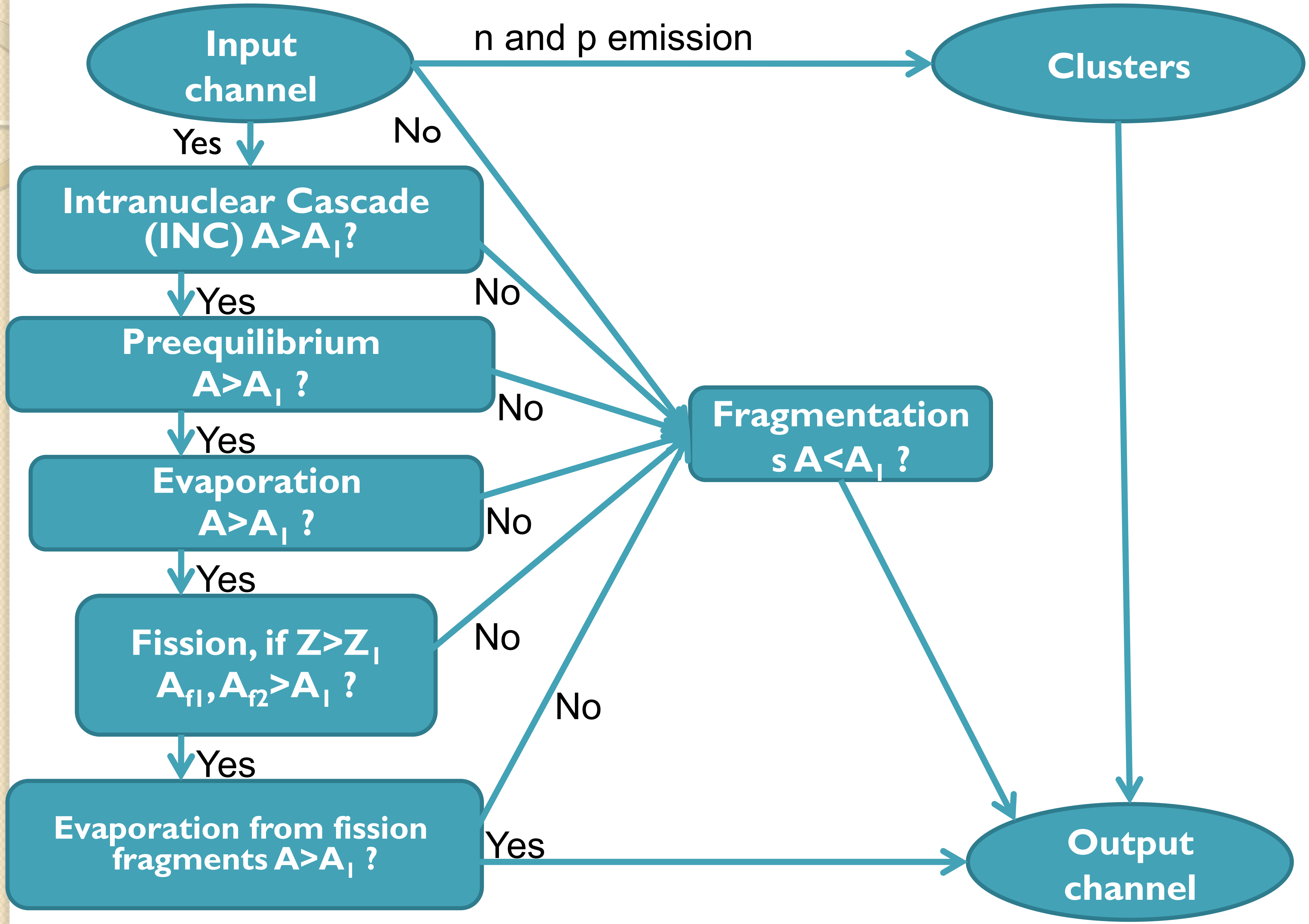
Library	Proton data		Neutron data	
	Number of files / Nuclear charge number range	Primary proton energy range	Number of files / Nuclear charge number range	Primary neutron energy range
The European Activation File, EAF-2007	816/1-100	up to 60 MeV	816/1-100	up to 60 MeV
Proton Activation Data File, PADF-2007	2355/12-88	up to 150 MeV	-	-
JENDL High Energy File 2007, JENDL/HE-2007	106/1-95	up to 3 GeV	106/1-95	up to 3 GeV
Joint Evaluated Fission and Fusion File, JEFF	26/20-83	up to 200 MeV	774/1-100	up to 20 MeV
TALYS-based Evaluated Nuclear Data Library, TENDL-2008	350/9-84	up to 200 MeV	350/9-84	up to 200 MeV
Medium Energy Nuclear Data Library, MENDL-2	-	-	505/13-84	up to 100 MeV
HEPAD-2008 library (INPE)				
High-Energy Proton Activation Data, HEPAD-2008	682/1-84	up to 1 GeV	-	-
IEAF-2005-rev1 library (INPE)				
The Intermediate Energy Activation File, IEAF-2005-rev1	-	-	682/1-84	up to 1 GeV

DIFFERENT APPROACHES TO THE SIMULATION OF THE HIGH-ENERGY INTERACTIONS

Approaches	Advantages	Disadvantages
Quantum molecular dynamics (QMD)	Only one model and nothing free parameters. Good correlation with experiments in the energy range high than 100÷1000 A×MeV.	Cannot be applied to the reaction up to E_0~100÷1000 A×MeV because of the shell effects influence on the interaction dynamics and initial configuration instability. **Linkage problem.**
Semiempirical	Short calculation time. Can be applying to the preliminary analysis.	Nothing simulations, only extrapolations of the experimental data.
Phenomenological	Good correlation with experiments in the energy range below 250-300 MeV.	Cannot be apply to the reaction in the energy range high than 3-4 GeV because of multiparticle interaction. There are a lot of different models depend on energy. **Free parameter variation problem.**

Our choice to the HEAD-2009 calculations

A GENERAL SCHEME OF THE CASCADE/PREEQUILIBRIUM/ EQUILIBRIUM CALCULATION

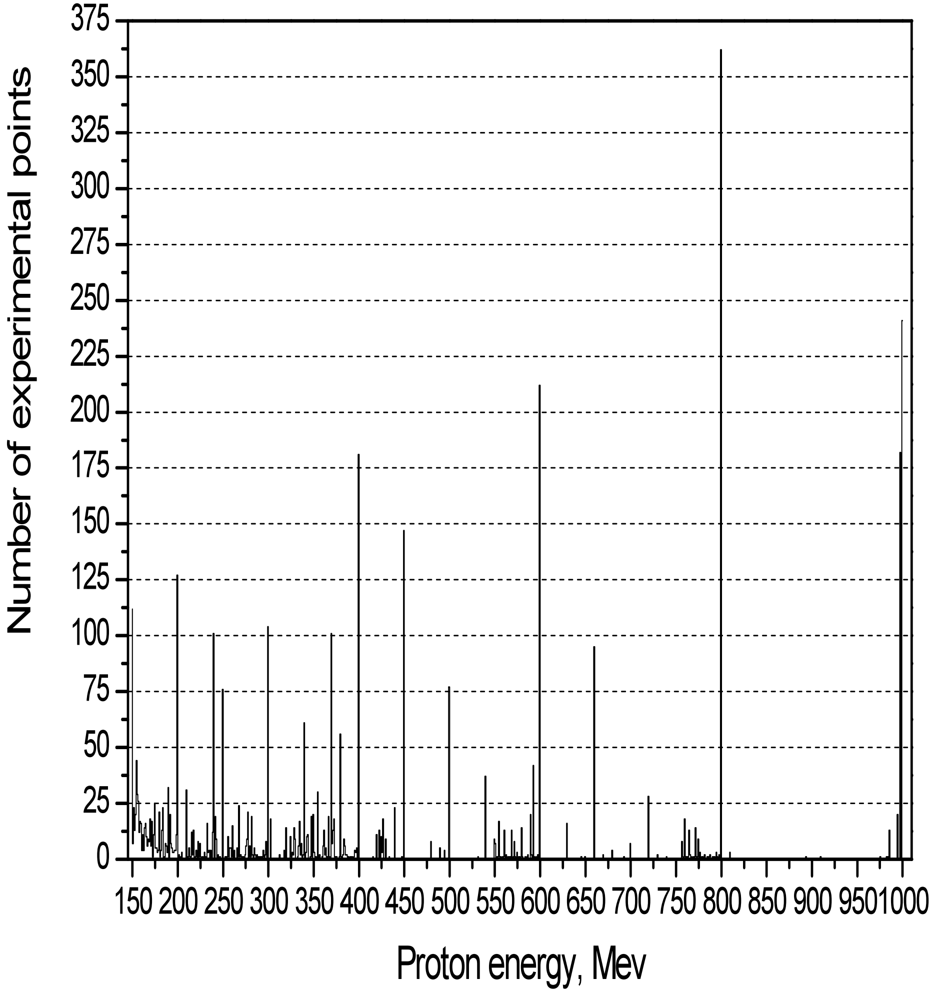


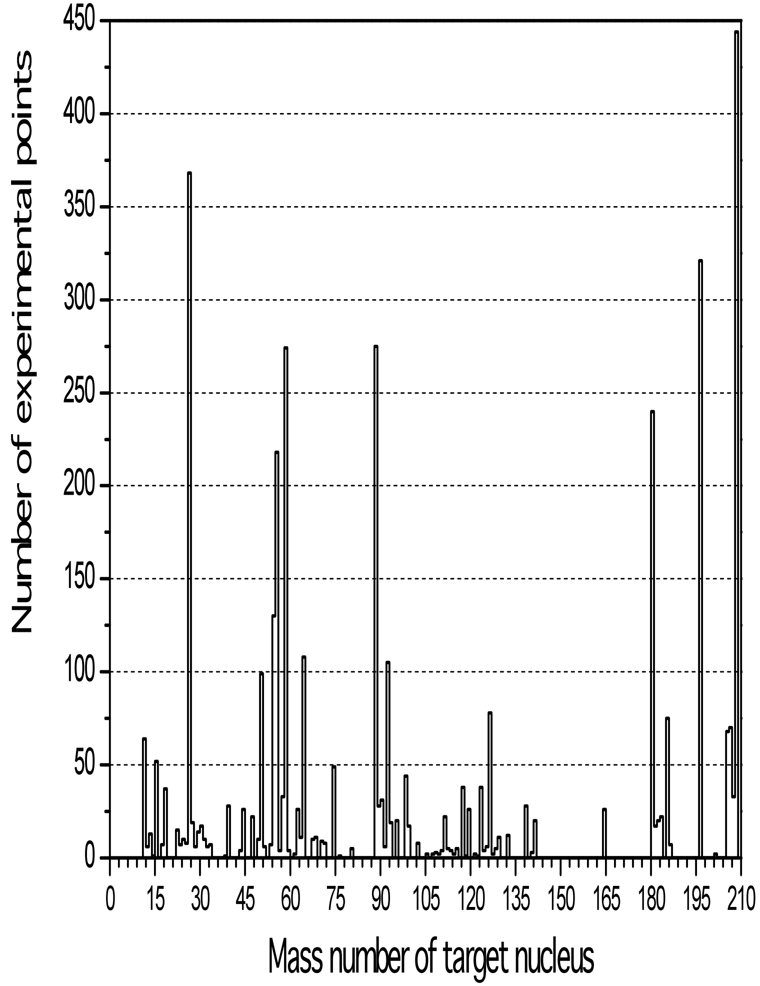
CRITERIA FOR COMPARISON OF INTRANUCLEAR CASCADE MODELS (MODEL ARBITRARY PARAMETERS) Expert approach:

- Nuclear density distribution (Bertini, ISABEL incorrectly).
- Pion potential and pion dynamics (Bertini и ISABEL incorrectly).
- Interactions between cascade particles (ISABEL, INCL4 and CASCADE take into account, in connection with Monte Carlo technique).
- Clusters (INCL4, CEM03.01 take into account).
- Effects of refractions and reflections at the nuclear surface (Bertini, ISABEL not take into account).
- Nuclear density depletion (Bertini not take into account).
- Monte Carlo technique (CASCADE, ISABEL and INCL4 the time-like Monte Carlo technique).
- The criterion to decide when a particle leaves the cascade stage (cutoff energy, expect INCL4 – stopping time).
- Fragmentation (CEM03.01).

CRITERIA FOR COMPARISON OF INTRANUCLEAR CASCADE MODELS (EXPERIMENTAL DATE BY EXFOR LIBRARY)

Statistical approach:





Distributions of experimental points for mass number of target nucleus and proton energy

Statistical approach (2)

- METHOD OF THE LEAST SQUARES;
- CORRELATION ANALISYS ;
- FACTOR ANALYSIS;
- REGRESSION ANALYSIS.

$$F = 10^{\sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(\lg\sigma_i^{\exp} - \lg\sigma_i^{calc}\right)^2}}$$

$$H = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(\frac{\sigma_i^{\exp} - \sigma_i^{cacl}}{\Delta\sigma_i^{\exp}}\right)^2}$$

N – the general numbers of experimental points,

$\sigma_i^{\exp}$ – experimental cross-section value

– calculation cross-section value

σ_i^{calc} – uncertainty of experimental cross-

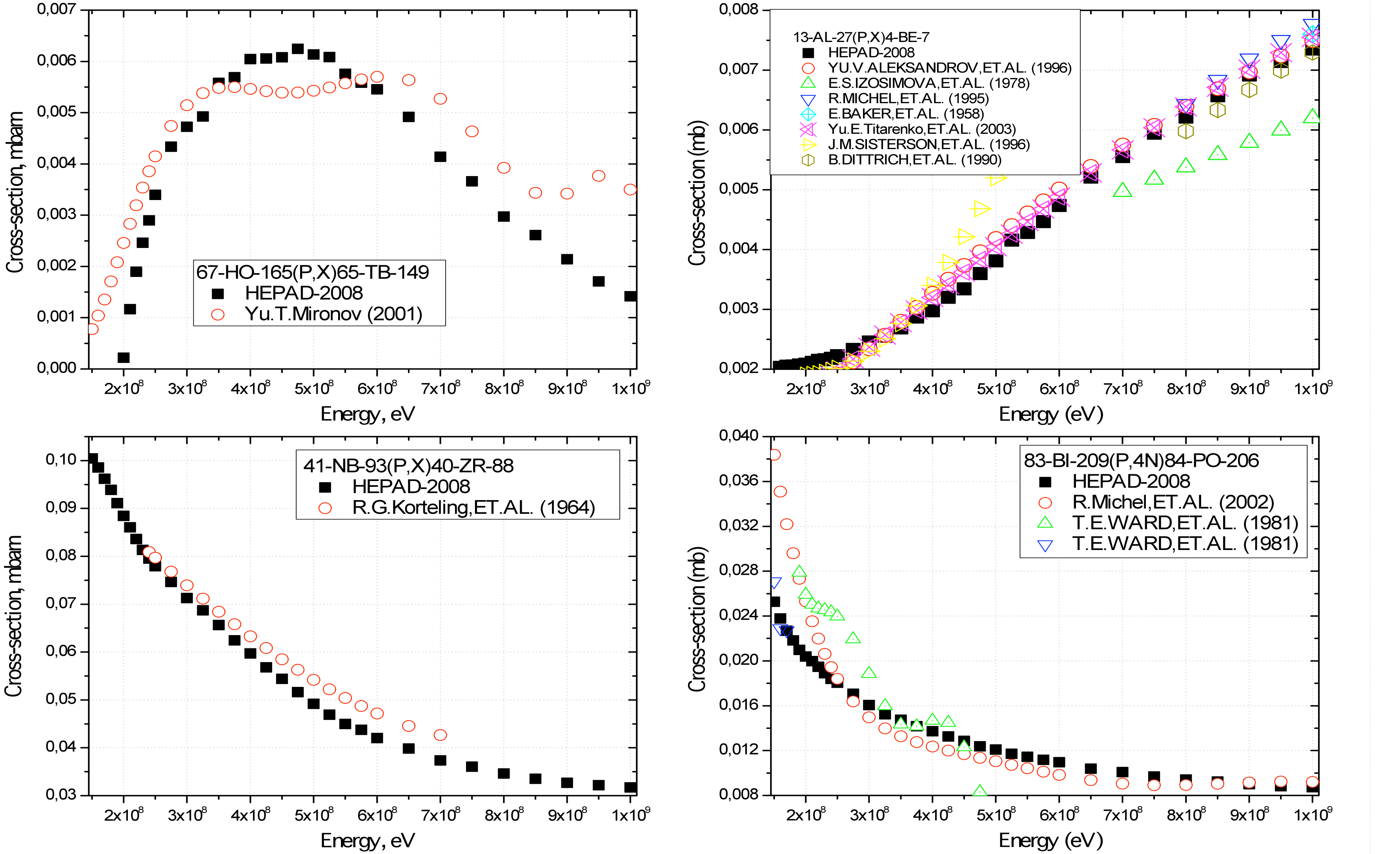
$\Delta\sigma_i^{\exp}$ section value

THE VALUES OF THE NORMALIZED LINEAR COMBINATION OF THE F- AND H- FACTORS DEPEND ON THE SUB-BANDS OF THE TARGET MASS NUMBER

Sub-bands of the target mass numbers	Bertini/ ABLA	Bertini/ Dresner	CEM03.01	INCL4/ ABLA	INCL4/ Dresner	ISABEL/ ABLA	ISABEL/ Dresner	CASCADE
12-19	0.3069	0.2931	**0.1818**	0.3660	0.3509	0.2583	0.2431	-
23-27	0.2730	0.1765	0.2784	0.3050	**0.1657**	0.3168	0.2232	0.2613
28-55	0.2820	0.2962	0.2123	0.2353	0.2379	0.2728	0.2898	**0.1736**
56-59	0.2442	**0.2170**	0.2354	0.2846	**0.2160**	0.2799	0.2436	0.2793
60-89	0.3001	0.3157	0.1814	0.2814	0.2933	0.2461	0.2413	**0.1406**
90-124	0.3523	0.2132	0.3371	0.2448	**0.1747**	0.2738	0.2175	0.1865
125-181	0.2634	0.2800	0.2312	0.2642	0.2738	0.2415	0.2362	**0.2096**
182-197	0.3092	0.3078	**0.1373**	0.3055	0.3189	0.2275	0.2515	0.1424
206-209	0.2849	0.3176	**0.1597**	0.2525	0.2952	0.2224	0.2700	0.1978

High Energy Proton Activation Data Library (HEPAD-2008)

Comparison between EXFOR and HEPAD-2008 data



Residual ^{149}Tb (top) and ^{88}Zr (bottom) production from ^{165}Ho(P,X) and ^{93}Nb(P,X) reactions respectively.

Residual ^{7}Be (top) and ^{206}Po (bottom) production from ^{27}Al(P,X) and ^{209}Bi(P,4N) reactions respectively.

THE CHANGES IN THE CEM03.01 MODEL IN COMPARISON WITH THE PREVIOUS VERSION

- new approximations for the total elementary cross sections have been developed;
- the possibility of cluster formation at the cascade stage was implemented;
- the condition for transition from the INC stage of a reaction to preequilibrium was changed; on the whole, the INC stage in CEM03.01 is longer, whereas the preequilibrium stage is shorter in comparison with the previous versions;
- the modified exciton model of the multiparticle preequilibrium decay was applied;
- the evaporation stage of reactions is calculated with an improved version of the Generalized Evaporation Model (GEM2) by Furihata;
- the fragmentation of light nuclei by using the Fermi break-up model is considered (CEM03.01 is the only model today which allows calculations for light nuclei (lighter lithium) to be made, the CASCADE/INPE code is not able to perform such calculations, either).

MODELS RECOMMENDED ON THE BASIS OF STATISTICAL ANALYSIS AND USED IN THE IEAF-2005 AND HEPAD-2008 LIBRARIES CALCULATIONS

Mass target range	Models for the IEAF-2005 calculation	Models for the HEPAD-2008 calculation
1-H-1 – 2-He-4	MCNPX interpolation tables	CEM03.01
3-Li-6 – 10-Ne-22	ISABEL/ Dresner	CEM03.01
11-Na-23 – 13-Al-27	*INCL4/Dresner*	*INCL4/Dresner*
12-Mg-28 – 27-Co-55	*CASCADE*	*CASCADE*
29-Cu-56 – 28-Ni-59	*Bertini/ Dresner*	*Bertini/Dresner*
26-Fe-60 – 40-Zr-89	*CASCADE*	*CASCADE*
38-Sr-90 – 54-Xe-124	*INCL4/ Dresner*	*INCL4/ Dresner*
50-Sn-125 – 75-Re-181	CEM2K	CASCADE
72-Hf-182 – 84-Po-210	CASCADE	CEM03.01

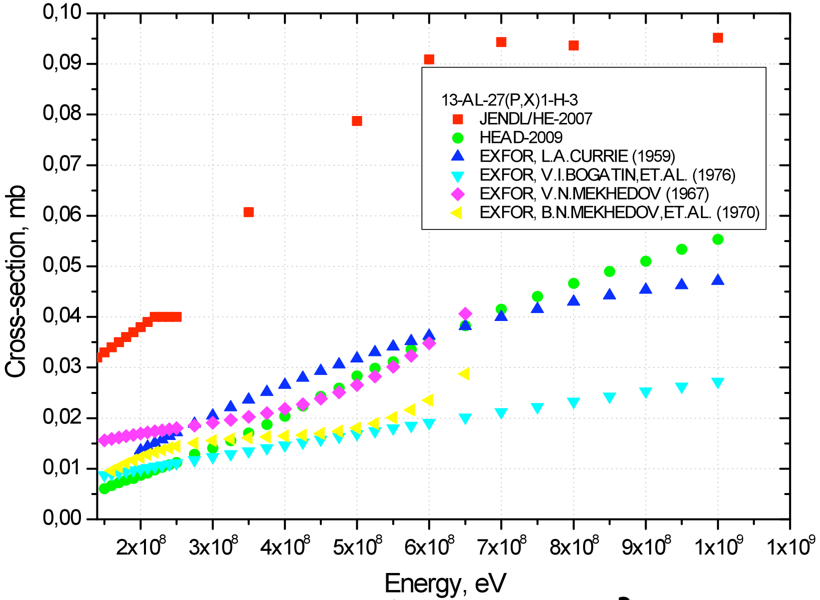
Values of the linear combination of normalized deviation factors H and F depending on the sub-band of target mass numbers for the IAEF-2005 library

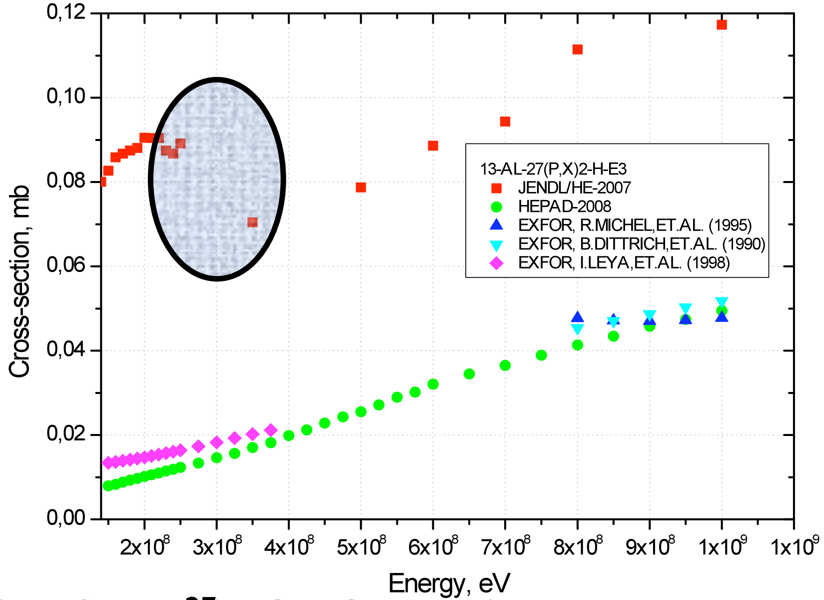
Target mass number sub-bands	Bertini/ ABLA	Bertini/ Dresner	CEM2K	INCL4/ ABLA	INCL4/ Dresner	ISABEL/ ABLA	ISABEL/ Dresner	CASCADE
12-19	0.022	0.020	**0.014**	0.030	0.028	0.016	**0.014**	
125-181	0.018	0.019	**0.011**	0.018	0.018	0.015	0.014	**0.010**
182-197	0.019	0.023	0.009	0.018	0.026	0.011	0.015	**0.005**
206-209	0.017	0.021	0.020	0.013	0.019	0.010	0.015	**0.008**

Values of the linear combination of normalized deviation factors H and F depending on the sub-band of target mass numbers for the HEPAD-2008 library

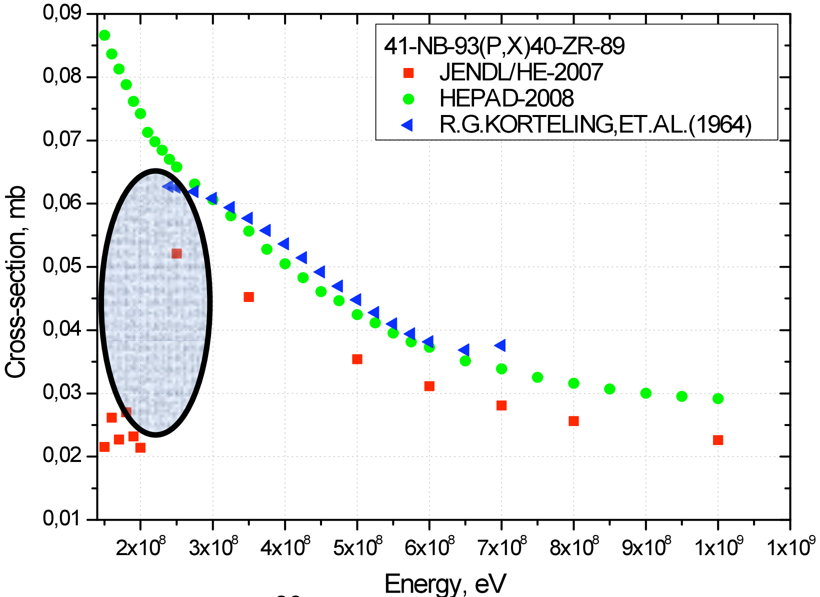
Target mass number sub-bands	Bertini/ ABLA	Bertini/ Dresner	CEM03.01	INCL4/ ABLA	INCL4/ Dresner	ISABEL/ ABLA	ISABEL/ Dresner	CASCADE
12-19	0.0236	0.0215	**0.0078**	0.0327	0.0301	0.0164	0.0145	
125-181	0.0172	0.0193	**0.0113**	0.0172	0.0180	0.0146	0.0139	**0.0103**
182-197	0.0233	0.0236	**0.0041**	0.0223	0.0254	0.0129	0.0154	**0.0042**
206-209	0.0203	0.0252	**0.0063**	0.0149	0.0215	0.0123	0.0177	0.0090

EXFOR, JENDL/HE-2007, HEAD-2009 COMPARISON

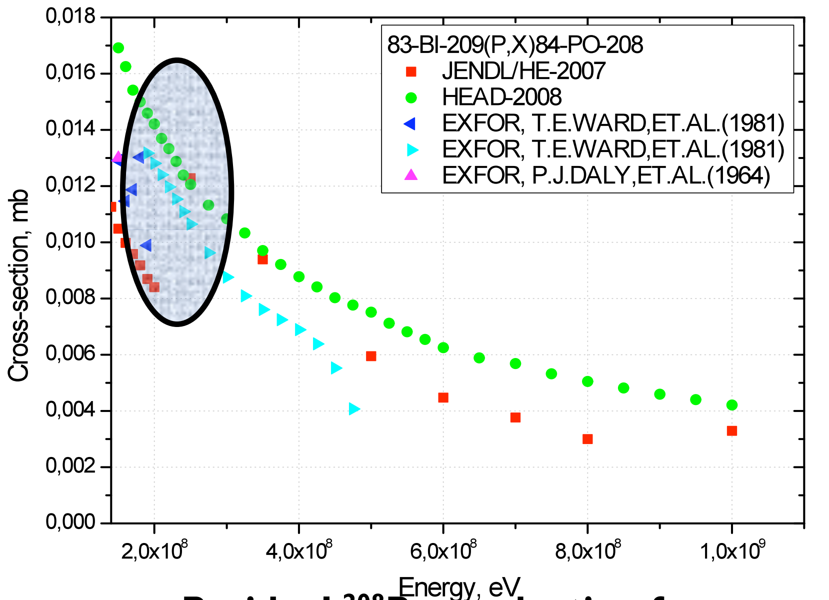




Residual t and ^{3}He production from ^{27}Al(P,X) reaction



Residual ^{89}Zr production from ^{93}Nb(P,X) reaction



Residual ^{208}Po production from ^{209}Bi(P,X) reaction

ADR Graphical user interface

STEP I (required)

Select the target isotope

STEP II (required)

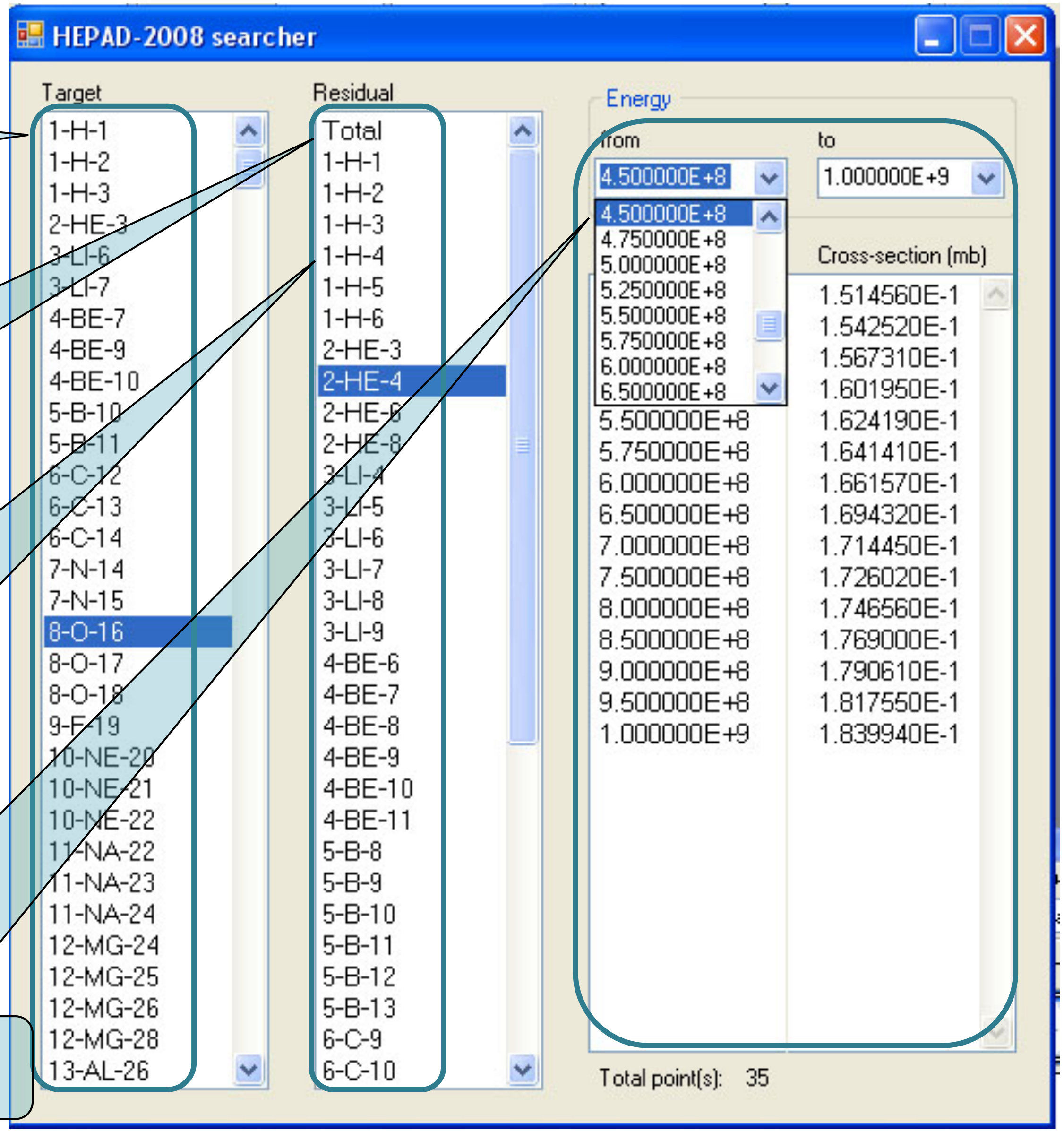
Select the total NON-elastic cross-section

or

Select the residual cross-section

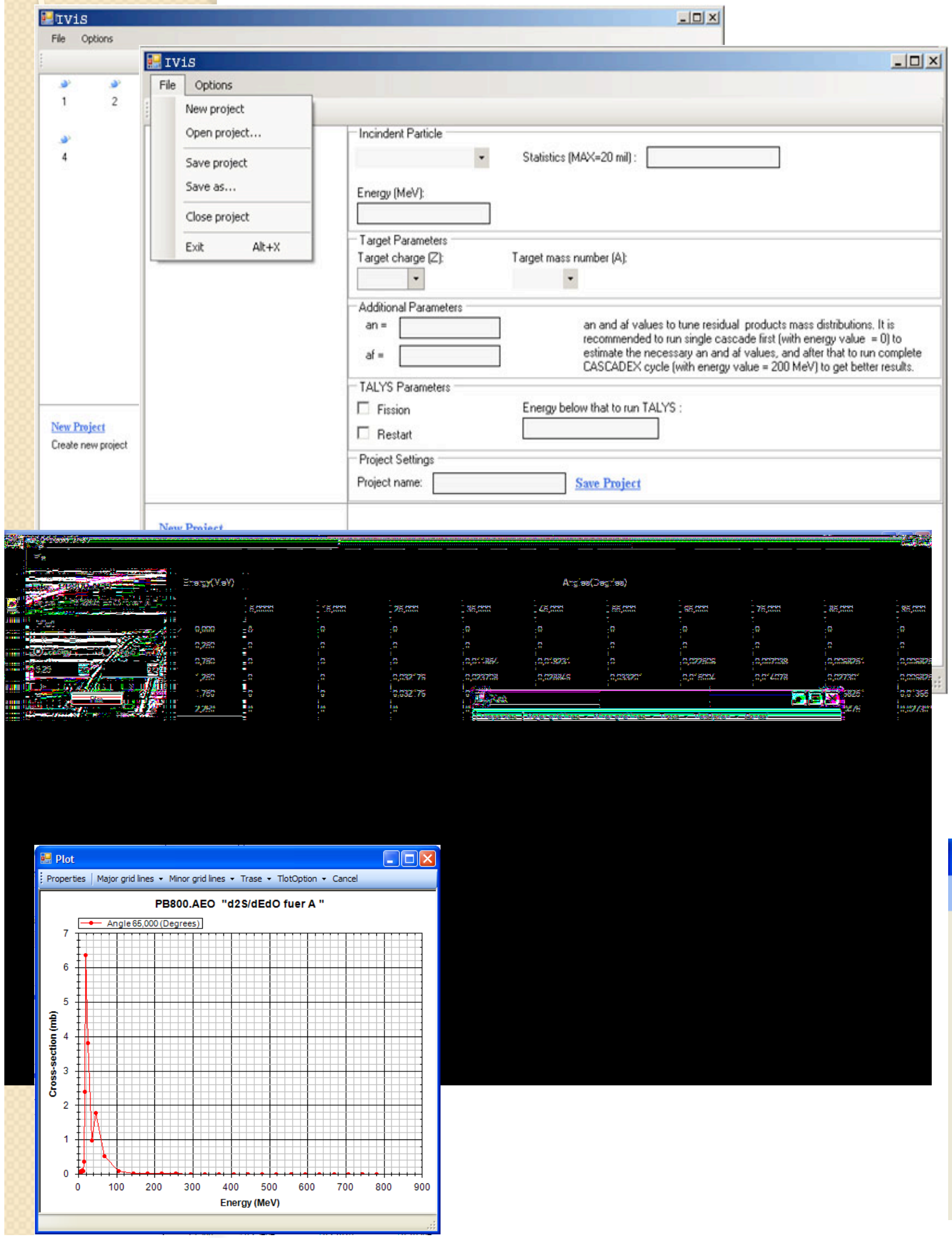
STEP III (optional)

Select the energy range

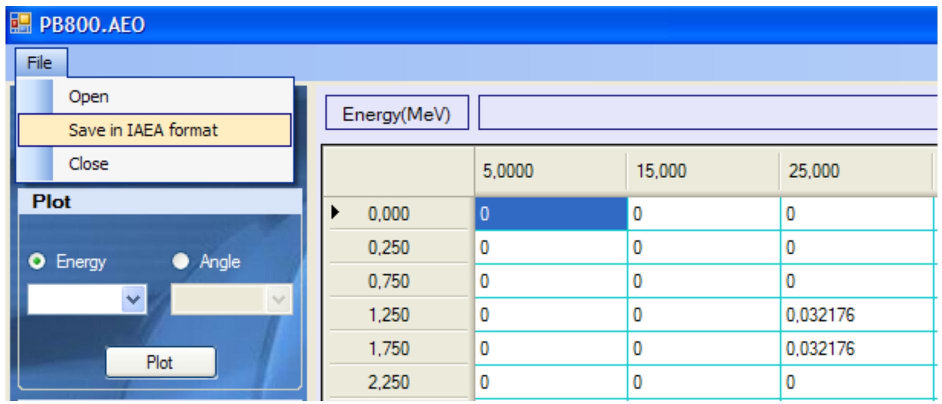


INTERACTIVE INFORMATIONAL SYSTEM FOR PREPARATION AND STATISTICAL ANALYSIS OF HIGH-ENERGY NUCLEAR DATA

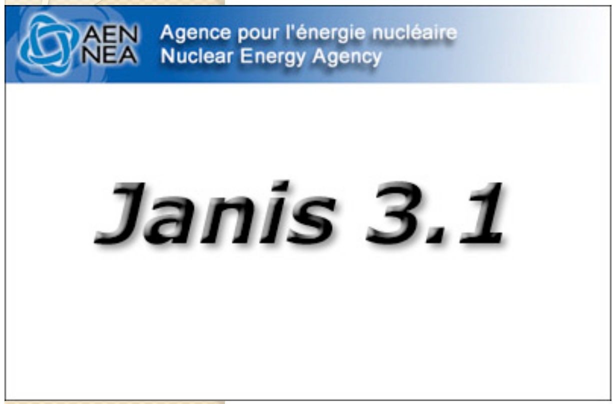
IVIS (interactive Visual System) for CASCADeX (CASCADeX GUI)



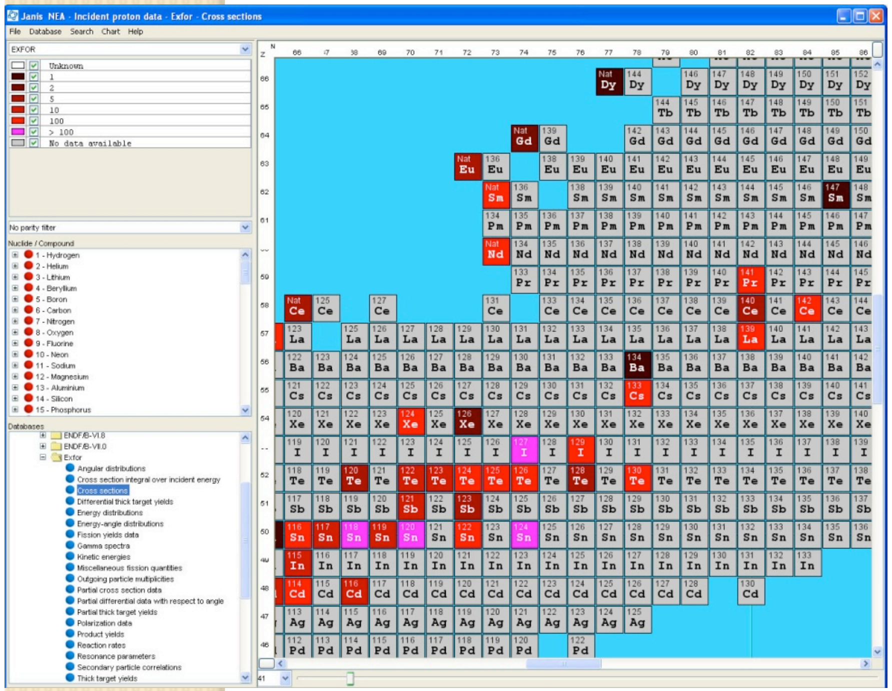
- Automated calculation
- Store data and provide easy access
- Visualization
- Data search
- Analyze data (Find better parameters of CascadEX code)

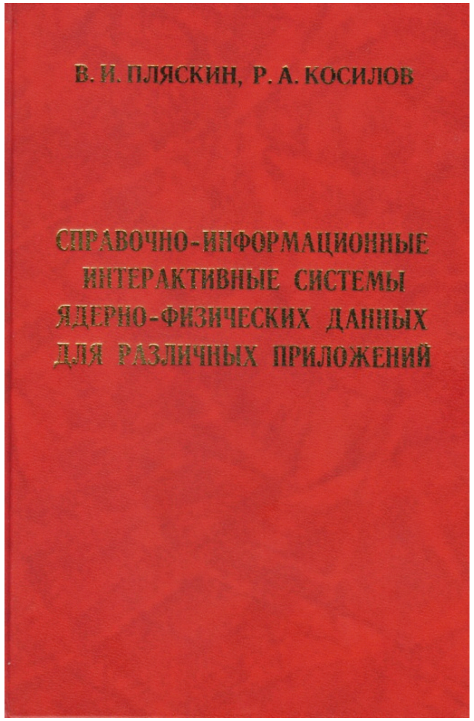


Examples of nuclear information software for data preparation



JANIS – JANIS (Java-based nuclear information software) is a display program designed to facilitate the visualization and manipulation of nuclear data. Its objective is to allow the user of nuclear data to access numerical values and graphical representations without prior knowledge of the storage format. It offers maximum flexibility for the comparison of different nuclear data sets.



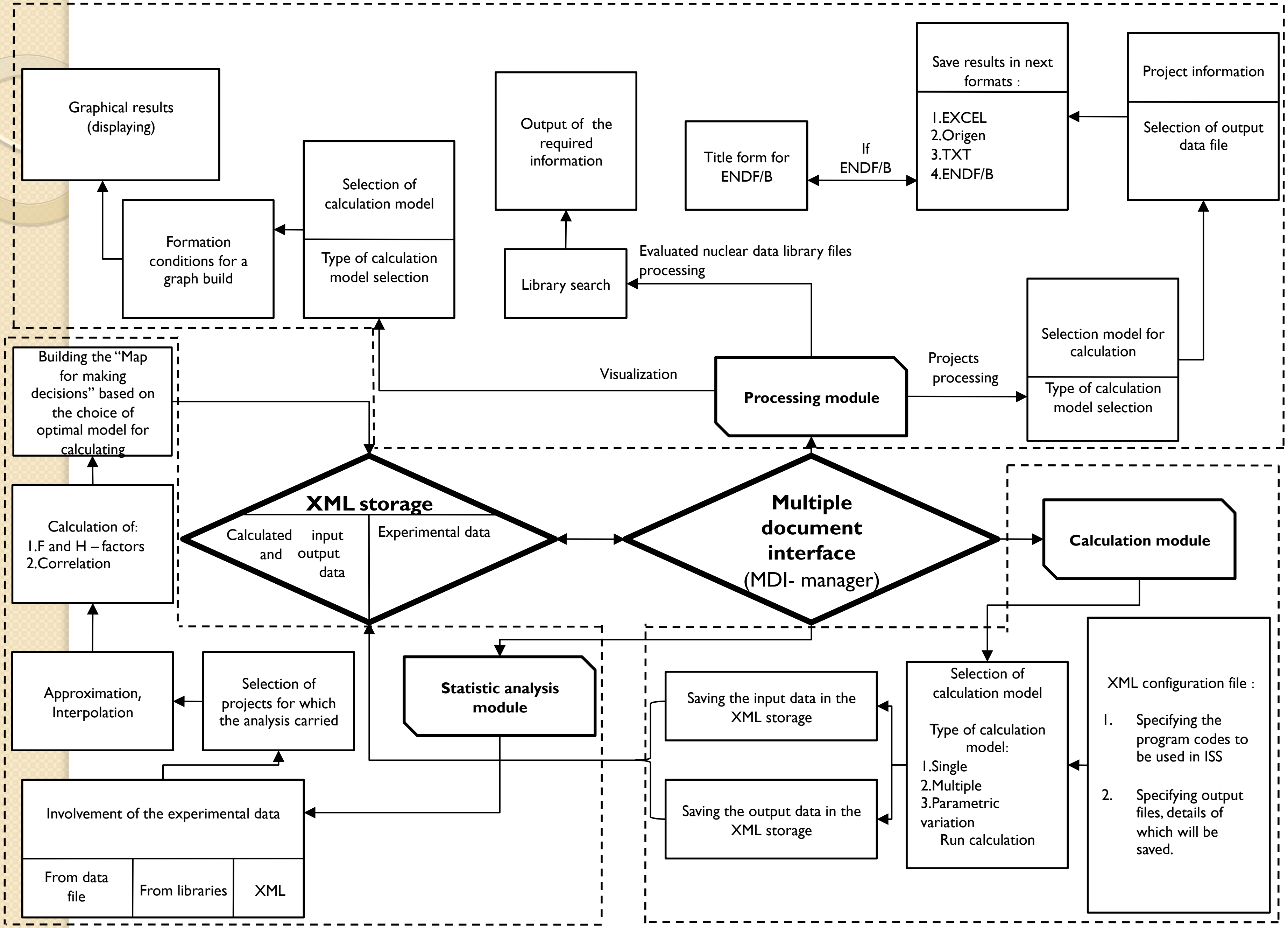


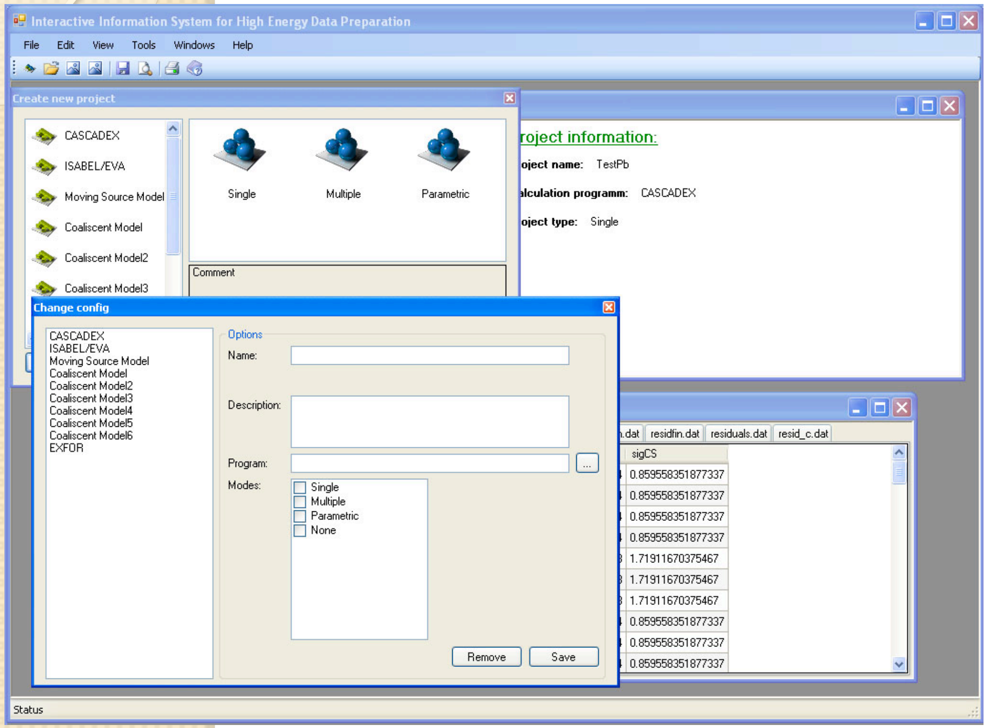
Information-Interactive System Software for low energy data preparation made by V.I. Plaskin and R.A. Kosilov. The advantages of this system is that the low energy nuclear data is combined with different useful calculations. ????

Current state of ISS

- Interactive shell that combines high-energy nuclear data library (HEPAD, TREF, IEAF, etc.)
- Models for calculations of high energy nuclear interactions (CASCAD, CASCADeX, DISCA, ISABEL / EVA, etc.) and the experimental data in the high-energy range (EXFOR)
- Moving source and coalescence models for calculation of double differential cross-sections
- Envisaged the possibility to import results in software packages Ecxel, Mathcad, Statistics, Origen with a view to their subsequent processing and graphical representation of nuclear data.

Scheme of ISS



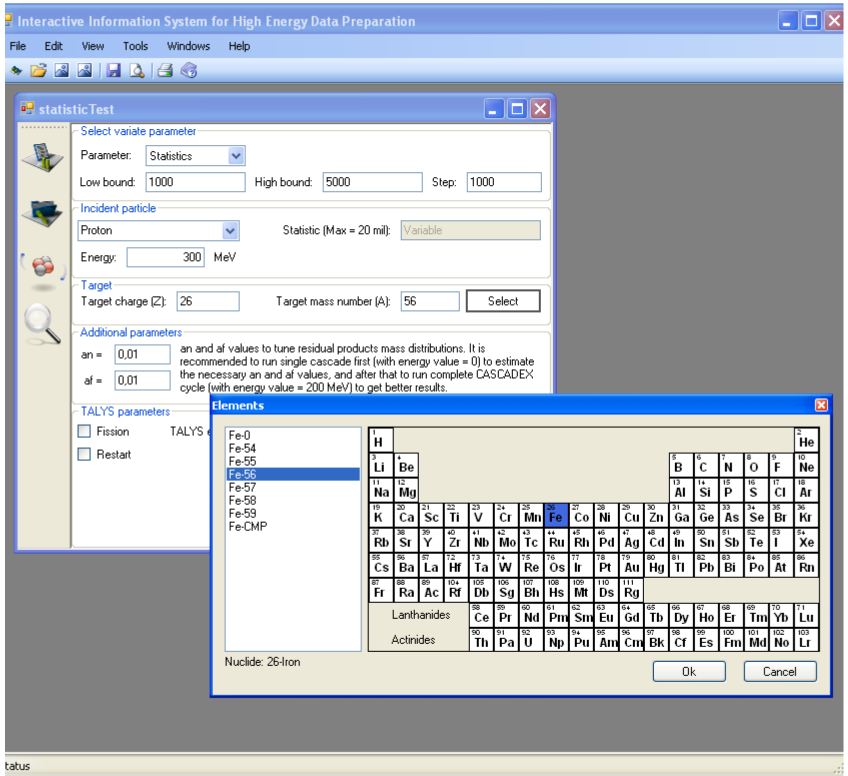


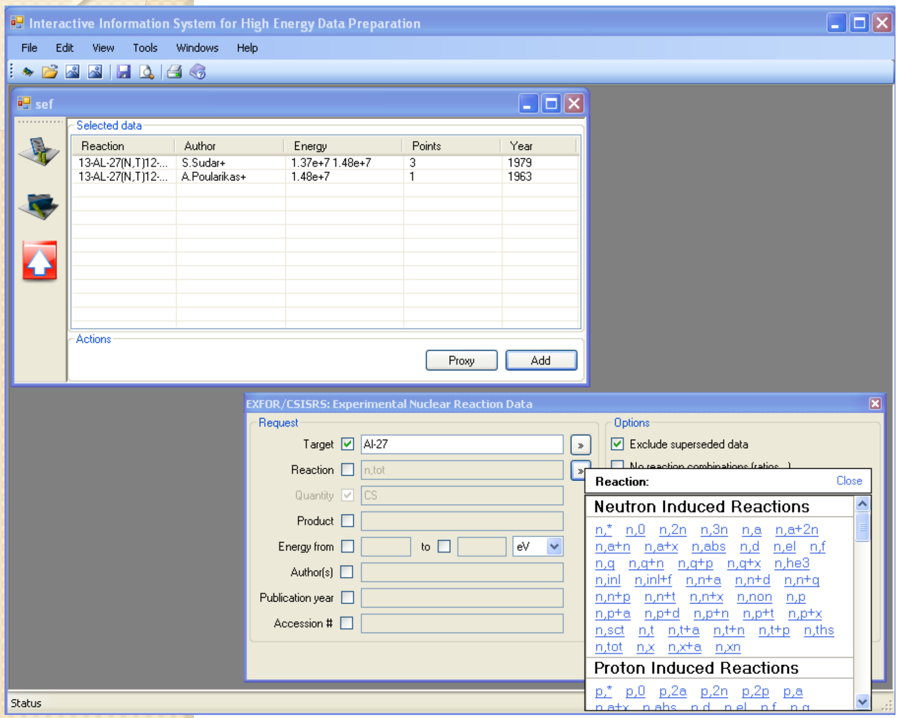
- Multi Document Interface (MDI-manager) allows you to work simultaneously on several parallel tasks

- Friendly user interface

- IIS giving the user ability to perform calculations with a variation of almost any parameters.

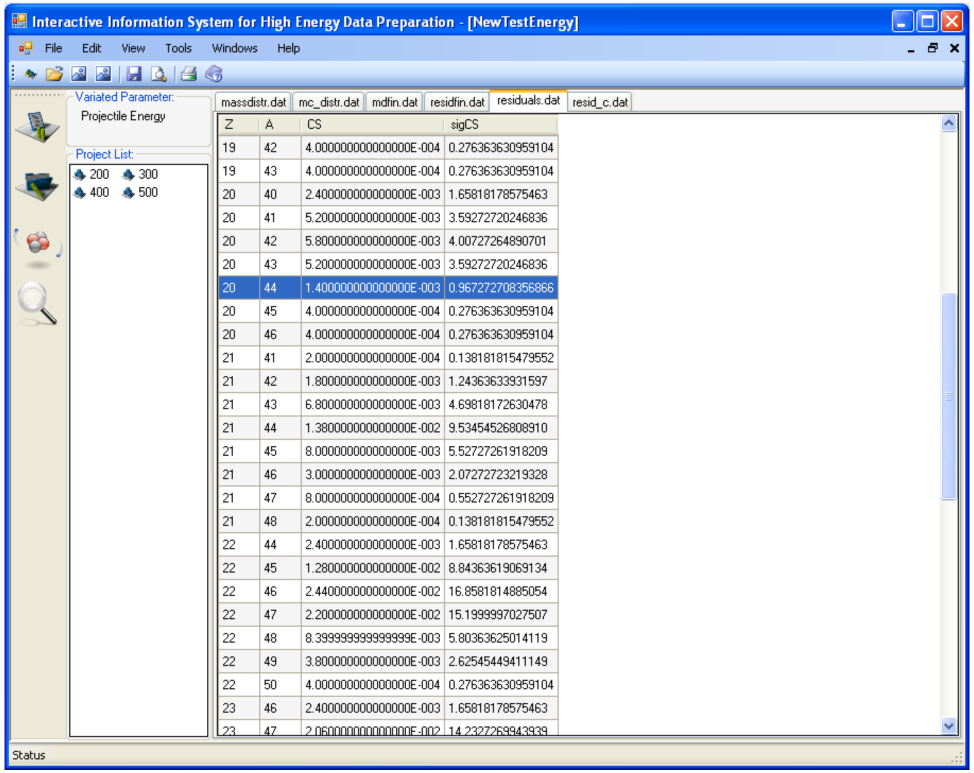
- Storage and access to data via XML - Storage

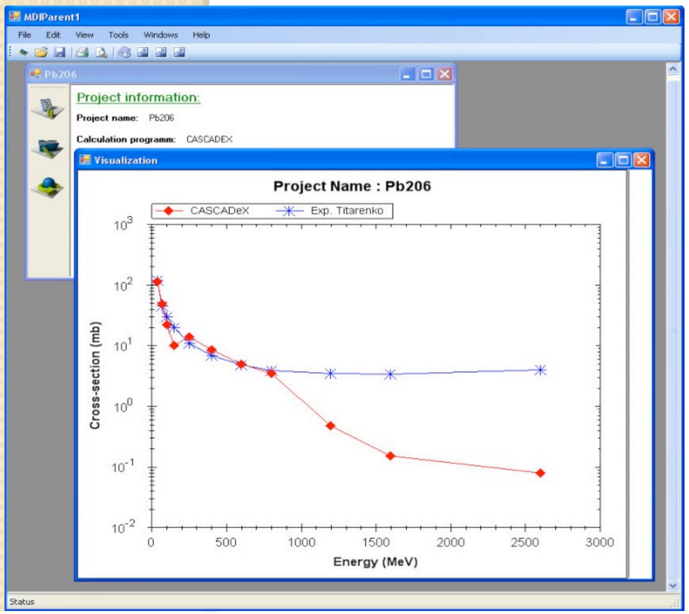




Easy access to any data

Automatic connection and preservation of experimental data from EXFOR Library





Data visualization

STATISTICAL ANALYSIS IN ISS

Correlation and Standard Deviation

Models comparing, selected by the values of criteria, have been conducted on the degree of correlation and standard deviation. This also enabled us to understand is this a good match models with experiments not accidental.

$$r_{xy} = \frac{\mu_{xy}}{(\sigma_x \sigma_y)}$$

, where

$$\mu_{xy} = M\{[X - M(X)][Y - M(Y)]\}$$

Standard deviation :

$$S = \sqrt{\frac{1}{m \cdot n} \sum_{i=0}^{n-1} \sum_{j=0}^{m-1} \left| M_{i,j} - \overline{M} \right|^2}$$

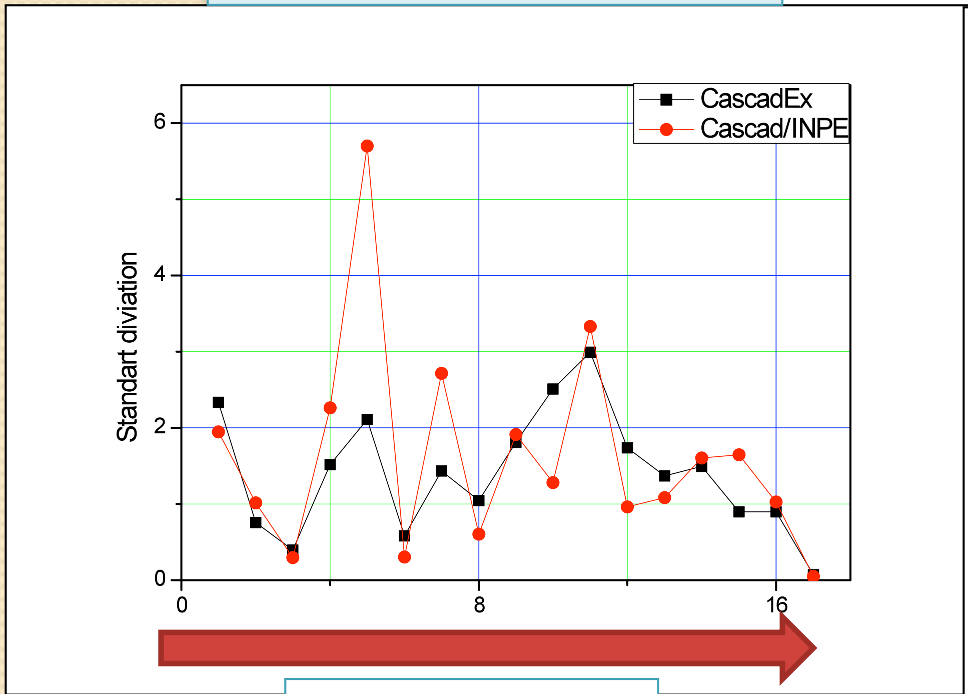
Correlation :

$$cor = \frac{\frac{1}{N} \cdot \sum_{i=0}^{N-1} (\sigma_i^{exp} - \langle \sigma^{exp} \rangle) \cdot (\sigma_i^{calc} - \langle \sigma^{calc} \rangle)}{\frac{1}{N} \cdot \sum_{i=0}^{N-1} (\sigma_i^{exp} - \langle \sigma^{exp} \rangle) \cdot \frac{1}{N} \cdot \sum_{i=0}^{N-1} (\sigma_i^{calc} - \langle \sigma^{calc} \rangle)},$$

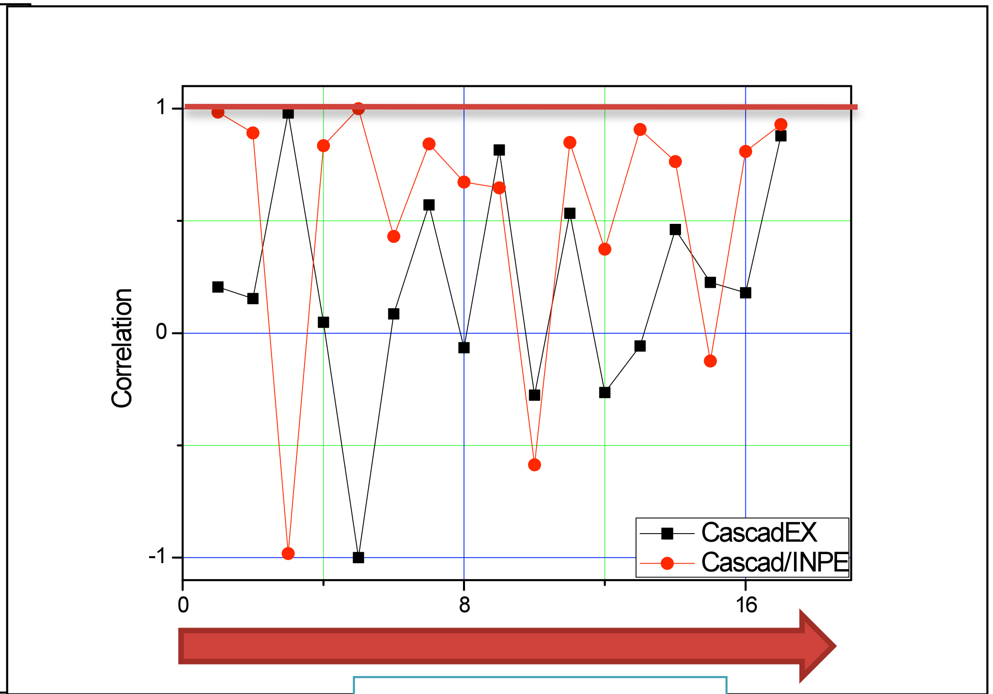
http://slovari.yandex.ru/dict/bse/article/00037/76400.htm

Example of Statistical Analysis of CASCADE and CASCADEX calculations for ^{206}Pb. (Correlation and Standard Deviation)

^{206}Pb - exp. Titarenko



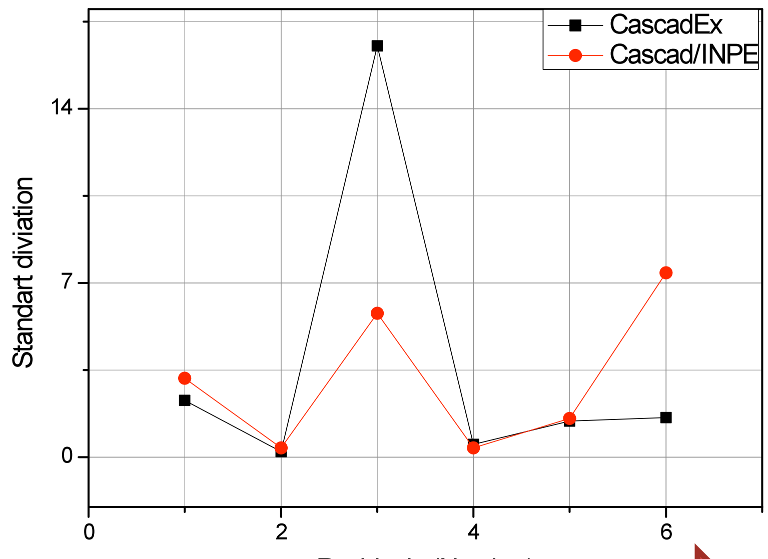
Increasing Z, A

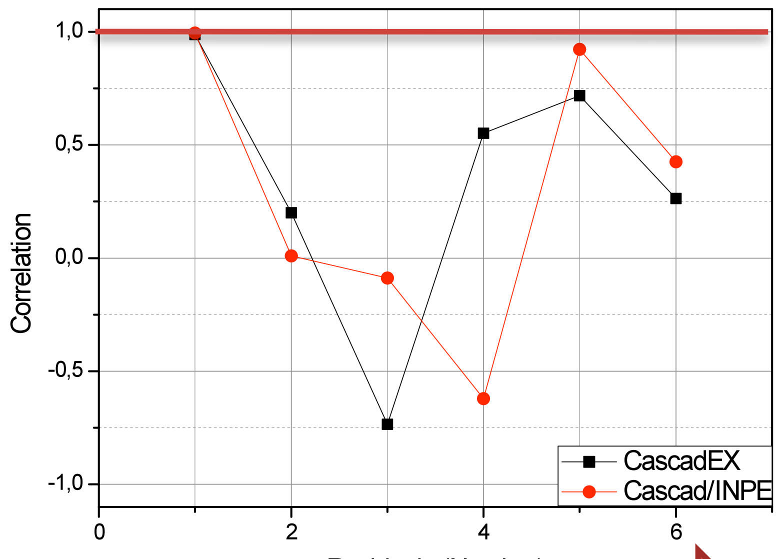


Increasing Z, A

Example of Statistical Analysis of CASCADE and CASCADEX calculations for ^{56}Fe. (Correlation and Standard Deviation)

^{56}Fe - exp. R. Michel





Increasing Z,A

Increasing Z,A

- IVIS CASCADeX is a flexible- intellectual system that allows user make a serial calculations based on CASCADEX with variation of free parameters (based on stochastic methods) in order to select the best model parameters for the comparison with experimental data.
- ISS represent the integration environment for cross-verification of different nuclear reactions models in order to select the best model by multivariate analysis, taking into account uncertainty and provide the possibility of preparing the nuclear evaluated data libraries

Conclusion

- IVIS CASCADeX is a flexible- intellectual system that allows user make a serial calculations based on CASCADEX with variation of free parameters (based on stochastic methods) in order to select the best model parameters for the comparison with experimental data.
- ISS represent the integration environment for cross-verification of different nuclear reactions models in order to select the best model by multivariate analysis, taking into account uncertainty and provide the possibility of preparing the nuclear evaluated data libraries

The HEPAD-2008 proton activation nuclear data library was developed.

The revision of the IEAF-2005 neutron activation data library has been performed, a set of nuclides for which the cross-section data can be updated by using a more modern and improved model are specified, and the corresponding calculations have been made in this work.

The HEPAD-2008 proton activation nuclear data library and the updated IEAF-2005-rev1 (2009) neutron activation nuclear data library represent now the general high-energy activation data library HEAD-2009 (High Energy Activation Data Library).

THANK YOU FOR YOUR KIND ATTENTION !